SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: ANUMAN WALLY Examiner #: 75463 Date: 1212104 Art Unit: 1757 Phone Number 30 272-1337 Serial Number: 10/789566 Mail Box and Bldg/Room Location: 284 9064 Results Format Preferred (circle): PAPER DISK E-MAIL			
If more than one search is submitted, please prioritize searches in order of need.			
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.			
Title of Invention: Bib Sheet Assached			~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~
Inventors (please provide full names): _			10 00 1/1/20 C
Earliest Priority Filing Date:			· M. Ore
For Sequence Searches Only Please includ appropriate serial number.	e all pertinent information	(parent, child, divisional, or issued patent n	umbers) along with the
Plasi search Era	cmpd of E	ermula (I). Mank y	nc
	•		
**********************	******	************	
STAFF USE ONLY Searcher: Usha Shrestie	Type of Search	Vendors and cost where a	pplicable
	NA Sequence (#)		
Searcher Phone #:	AA Sequence (#)		
Searcher Location: Date Searcher Picked Up: 12 10 07	Structure (#) Bibliographic		
Date Completed: 12 10 04	Litigation		
Searcher Prep & Review Time: 50	Fulltext	Sequence Systems	
Clerical Prep Time:	Patent Family	· · · · · · · · · · · · · · · · · · ·	
Online Time: 200	Other	Other (specify)	

WHAT IS CLAIMED IS:

1. A compound represented by the formula

(I)

wherein:

 R_1 , R_2 , R_5 , R_6 , R_8 , R_9 and R_{10} are each independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, alkynyl, substituted alkynyl, heterocycloalkyl, substituted heterocycloalkyl, substituted carbonyl, acylamino, halogen, nitro, nitrilo, sulfonyl, aryl, substituted aryl, heteroaryl, substituted heteroaryl, oxygen, substituted oxygen, nitrogen, substituted nitrogen, sulfur and substituted sulfur;

 R_3 and R_4 are each independently selected from the group consisting of hydrogen, alkyl having from 1 to 3 carbon atoms, substituted alkyl having from 1 to 3 carbon atoms, alkenyl having from 1 to 3 carbon atoms, substituted alkenyl having from 1 to 3 carbon atoms,

alkynyl having from 1 to 3 carbon atoms, substituted alkynyl having from 1 to 3 carbon atoms, substituted oxygen, substituted nitrogen, and substituted sulfur;

R₇ is absent or selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, substituted alkynyl, heterocycloalkyl, substituted heterocycloalkyl, substituted carbonyl, acylamino, halogen, nitro, nitrilo, sulfonyl, aryl, substituted aryl, heteroaryl, substituted heteroaryl, oxygen, substituted oxygen, nitrogen, substituted nitrogen, sulfur and substituted sulfur;

R₁₁ is selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, alkenyl, substituted alkynyl, heterocycloalkyl, substituted heterocycloalkyl, substituted carbonyl, acylamino, sulfonyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl; and

X₁ is carbon or nitrogen;

provided that at least one of R_1 , R_2 , R_5 and R_6 is selected from the group consisting of alkyl, substituted alkyl, alkenyl, substituted alkenyl, alkynyl, substituted alkynyl, heterocycloalkyl, substituted heterocycloalkyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl.

2. A compound according to Claim 1 wherein X_1 is carbon, R_7 , R_8 , R_9 and R_{10} are each hydrogen and R_1 , R_2 , R_3 , R_4 , R_5 , R_6 and R_{11} are as defined in Claim 1.

- 3. A compound according to Claim 1 wherein R_{11} is alkyl or substituted and two of R_1 , R_2 , R_5 and R_6 are alkyl or substituted alkyl having between one and twelve carbon atoms and X_1 is carbon.
- 4. A compound according to Claim 1 wherein R_1 , R_3 , R_4 , R_6 , R_7 , R_8 , R_9 and R_{10} are each hydrogen, R_2 and R_5 are each alkyl having 6 carbon atoms, R_{11} is ethyl and X_1 is carbon.
- 5. A compound according to Claim 1 wherein R_1 , R_3 , R_4 , R_6 , R_7 , R_8 , R_9 and R_{10} are each hydrogen, R_2 and R_5 are each alkyl having 3 carbon atoms, R_{11} is benzyl and X is carbon.
- 6. A compound according to Claim 1 wherein R_1 , R_3 , R_4 , R_6 , R_7 , R_8 , R_9 and R_{10} are each hydrogen, R_2 and R_5 are each benzyl, R_{11} is $-CH_2CH_2CH_3)_2$, and X_1 is carbon.
- 7. A color imaging member comprising a first image-forming layer including a compound according to Claim 1, said compound being in the crystalline form.
- 8. The imaging member as defined in Claim 7 and further including a substrate and at least a second color-forming layer, said second color-forming layer being capable of forming a color different from that formed by said first color-forming layer.

- 9. The imaging member as defined in Claim 8 and further including a third color-forming layer, said third color-forming layer being capable of forming a color different from those formed by said first and second color-forming layers.
- 10. The imaging member as defined in Claim 9 wherein said color-forming layers form magenta, cyan and yellow color, respectively.
 - 11. An imaging method comprising
- (a) providing an imaging member as defined in Claim 7; and
- (b) converting at least a portion of said compound to the liquid form in an imagewise pattern whereby an image is formed.
- 12. The method as defined in Claim 11 wherein step(b) comprises applying an imagewise pattern of thermal energy to said imaging member whereby at least a portion of said compound is converted to the liquid form and an image is formed.
- 13. The imaging method as defined in Claim 12 wherein said imaging member further includes a substrate and at least a second color-forming layer, said second color-forming layer being capable of forming a color different from that formed by said first color-forming layer.

- 14. The imaging method as defined in Claim
 13 wherein said imaging member further includes a third
 color-forming layer, said third color-forming layer
 being capable of forming a color different from those
 formed by said first and second color-forming layers.
- 15. The imaging method as defined in Claim 14 wherein said color-forming layers form magenta, cyan and yellow color, respectively.

0/789566

Classification: 430/357.000 Inventor: CHEON, KAP-SOO, et al Status: 30 - DOCKETED NEW CASE - READY FOR EXAMINATION Title: NOVEL DYES AND USE THEREOF IN IMAGING MEMBERS AND METHODS Examiner: WALKE, AMANDA

GAU: 1752

Bib Data report

Application Title: NOVEL DYES AND USE THEREOF IN IMAGING MEMBERS AND METHODS

Filing Date:02/27/2004 Application Num: (a) (in phx) 10789566 Effective Filing \mathfrak{D}2/27/2004

Foreign/Continuity Data) (Location History) Status: 30/DOCKETED NEW CASE - READY FOR EXAMINATION Status Date: 09/03/2004

Date of Abandonment: N/A PALM Location: Issue Date: N/A Confirmation Number:9239 Patent Number: Not Issued

Group Art Unit:1752 WALKE, AMANDA<u>Assignment Data</u> Class/Subclass: 430/357.000 Examiner: 75663

Total Claims: 15 Sheets/Drawing: 0 State or Country: MASSACHUSETTS Independent Claims: 1

MASSACHUSETTS **MASSACHUSETTS** MASSACHUSETTS MASSACHUSETTS Country or State: SHREWSBURY ARLINGTON ACTON MEDFIELD City: Last name, First name: FLFER STEPHEN CHEON. KAP-SOO ohu, Petier nventors:

Attorney Docket No:8586-AFP/GDM ALL Attorneys:

<WALKE 10/789566><Page 1>

=> fil reg FILE 'REGISTRY' ENTERED AT 14:46:09 ON 10 DEC 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

=> d his

```
FILE 'LREGISTRY' ENTERED AT 09:40:17 ON 10 DEC 2004
L1
               STR
L2
               STR L1
L3
               STR L1
L4
               STR L2
     FILE 'REGISTRY' ENTERED AT 10:54:42 ON 10 DEC 2004
L5
            50 S L4
L6
               STR L2
L7
            50 S L6
L8
          8631 S L6 FULL
               SAV L8 WAL566/A
     FILE 'HCAPLUS' ENTERED AT 11:37:04 ON 10 DEC 2004
L9
          1195 S CHEON ?/AU
         23478 S CHU ?/AU
L10
.L11
           128 S FILOSA ?/AU
           413 S TELFER ?/AU
L12
L13
            0 S L9 AND L10 AND L11 AND L12
   FILE 'HCAPLUS' ENTERED AT 11:57:48 ON 10 DEC 2004
L14
           57 S CHEON K?/AU
L15
         1169 S CHU P?/AU
L16
          128 S FILOSA ?/AU
L17
           413 S TELFER ?/AU
               S L1 AND L2 AND L3 AND L4
     FILE 'HCAPLUS' ENTERED AT 11:59:34 ON 10 DEC 2004
             0 S L14 AND L15 AND L16 AND L17
L18
             0 S L14 AND L15
L19
L20
             1 S L14 AND L16
             0 S L14 AND L17
L21
L22
            0 S L15 AND L16
            3 S L15 AND L17
3 S L16 AND L17
L23
L24
             7 S L18-L24
L25
               SEL L25 1-7 RN
```

<WALKE 10/789566><Page 2>

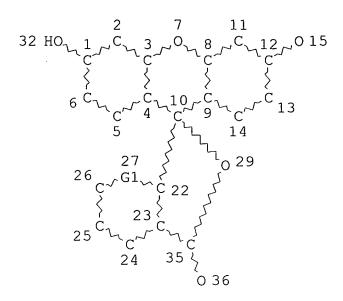
```
FILE 'REGISTRY' ENTERED AT 12:04:30 ON 10 DEC 2004
           272 S E1-E272
L26
            97 S C34H40O5
L27
L28
            1 S L26 AND L27
L29
        12534 S 7938.12.8/RID
L30
            36 S L29 AND L26
L31
             0 S L1 SSS SAM SUB=L8
L32
             STR L1
L33
            1 S L32 SSS SAM SUB=L8
L34
             2 S L32 SSS FUL SUB=L8
    FILE 'HCAPLUS' ENTERED AT 12:38:21 ON 10 DEC 2004
L35
            1 S L34
    FILE 'REGISTRY' ENTERED AT 12:40:54 ON 10 DEC 2004
              SAV L34 WAL566A/A
            50 S L3 SSS SAM SUB=L8
L36
L37
          6577 S L3 SSS FUL SUB=L8
              SAV L37 WAL566B/A
L38
             9 S L30 AND L37
    FILE 'CAOLD' ENTERED AT 13:07:30 ON 10 DEC 2004
L39
            0 S L34
L40
             0 S L38
    FILE 'HCAPLUS' ENTERED AT 13:07:58 ON 10 DEC 2004
L41
            1 S L38
             E OPTICAL IMAGING DEVICES/CV
L42
         31947 S E3
L43
        147550 S IMAGING#
L44
        352089 S DYE?
L45
        20476 S L37
           41 S L45 AND L42
L46
L47
           654 S L45 AND L43
L48
         6853 S L45 AND L44
L49
           41 S L46 AND L47
L50
           27 S L46 AND L48
L51
         ·240 S L47 AND L48
L52
            27 S L49 AND L51
    FILE 'HCAPLUS' ENTERED AT 13:17:44 ON 10 DEC 2004
L53
            27 S L51 AND L52
   FILE 'REGISTRY' ENTERED AT 13:18:37 ON 10 DEC 2004
L54
              STR L3
L55
            0 S L54 SSS SAM SUB=L37
L56
            0 S L54 SSS SAM SUB=L37
```

<WALKE 10/789566><Page 3>

```
L57
             1 S L54 SSS FUL SUB=L37
               SAV L57 WAL566C/A
     FILE 'HCAPLUS' ENTERED AT 13:26:11 ON 10 DEC 2004
L58
             1 S L57
     FILE 'LREGISTRY' ENTERED AT 13:27:40 ON 10 DEC 2004
L59
                STR L3
     FILE 'REGISTRY' ENTERED AT 14:04:20 ON 10 DEC 2004
L60
             0 S L59 SSS SAM SUB=L37
L61
                STR L59
L62
             0 S L61 SSS SAM SUB=L37
L63
               STR L61
L64
            50 S L63 SSS SAM SUB=L37
               STR L59
L65
L66
               STR L61
L67
             2 S L65 SSS SAM SUB=L37
L68
            37 S L65 SSS FUL SUB=L37
                SAV L68 WAL566D/A
     FILE 'HCAPLUS' ENTERED AT 14:16:49 ON 10 DEC 2004
L69
            34 S L68
     FILE 'REGISTRY' ENTERED AT 14:17:20 ON 10 DEC 2004
L70
              3 S L66 SSS SAM SUB=L37
L71
           110 S L66 SSS FUL SUB=L37
               SAV L71 WAL566E/A
    FILE 'HCAPLUS' ENTERED AT 14:19:13 ON 10 DEC 2004
L72
           66 S L71
L73
             1 S L72 AND L42
L74
             5 S L72 AND L43
L75 .
            34 S L72 AND L44
L76
             1 S L75 AND (L50 OR L52 OR L53)
         875772 S OPTIC?
L77
L78
            14 S L72 AND L77
L79
            10 S L78 AND (L42 OR L43 OR L44)
L80
            18 S L41 OR L58 OR L73 OR L74 OR L76 OR L79 OR L78
           60 S (L50 OR L52 OR L53 OR L69)
L81
L82
           59 S (L50 OR L52 OR L53 OR L69) NOT L80
          21 S L75 NOT (L80 OR L82)
L83
=> d 157 que stat
```

L3

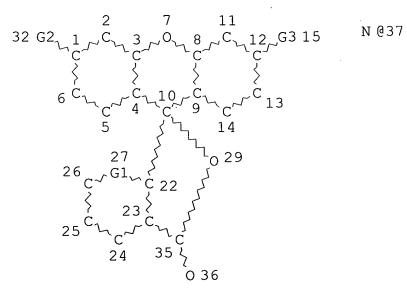
STR



VAR G1=C/N NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE L6 STR



VAR G1=C/N

VAR G2=N/O
VAR G3=O/37
NODE ATTRIBUTES:
NSPEC IS RC AT 37
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

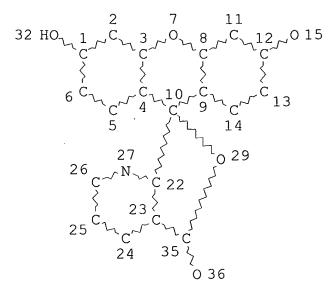
RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

L8 8631 SEA FILE=REGISTRY SSS FUL L6

L37 6577 SEA FILE=REGISTRY SUB=L8 SSS FUL L3

L54 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

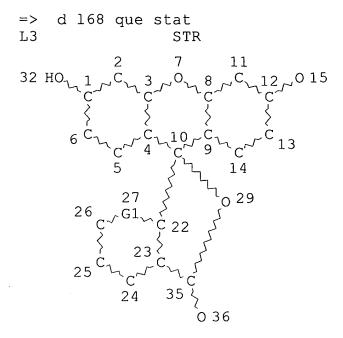
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L57 1 SEA FILE=REGISTRY SUB=L37 SSS FUL L54

100.0% PROCESSED 30 ITERATIONS 1 ANSWERS

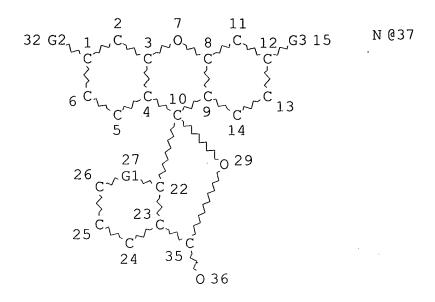
SEARCH TIME: 00.00.01



VAR G1=C/N NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE L6 STR



VAR G1=C/N
VAR G2=N/O
VAR G3=O/37
NODE ATTRIBUTES:
NSPEC IS RC AT 37
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 26

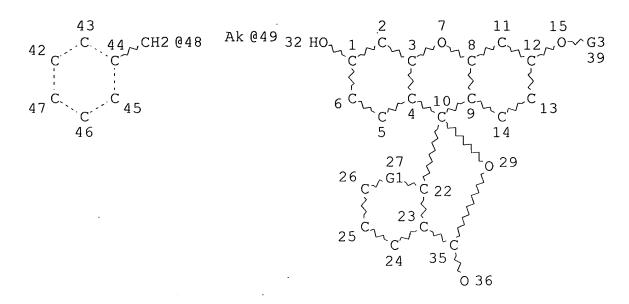
STEREO ATTRIBUTES: NONE

L8 8631 SEA FILE=REGISTRY SSS FUL L6

L37 6577 SEA FILE=REGISTRY SUB=L8 SSS FUL L3

L65 STR

<WALKE 10/789566><Page 8>



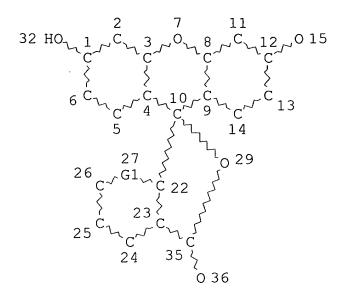
VAR G1=C/N
VAR G3=48/49
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 49
DEFAULT MLEVEL IS ATOM .
GGCAT IS SAT AT 49
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE
L68 37 SEA FILE=REGISTRY SUB=L37 SSS FUL L65

100.0% PROCESSED 6577 ITERATIONS 37 ANSWERS SEARCH TIME: 00.00.01

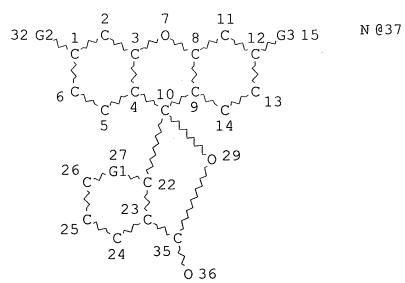
=> d 171 que stat L3 STR



VAR G1=C/N NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE L6 STR



<WALKE 10/789566><Page 10>

VAR G1=C/N
VAR G2=N/O
VAR G3=O/37
NODE ATTRIBUTES:
NSPEC IS RC AT 37
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

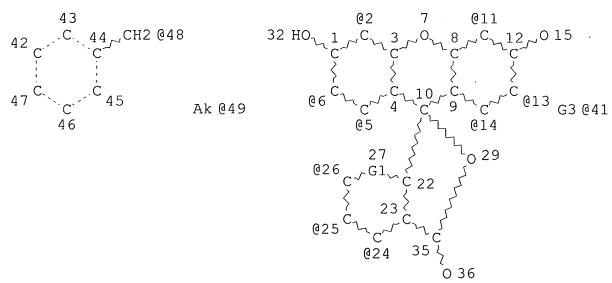
RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

L8 8631 SEA FILE=REGISTRY SSS FUL L6

L37 6577 SEA FILE=REGISTRY SUB=L8 SSS FUL L3

L66 STR



VAR G1=C/N
VAR G3=48/49
VPA 41-13/11/2/6/5/14/26/25/24 U
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 49
DEFAULT MLEVEL IS ATOM
GGCAT IS SAT AT 49
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L71 110 SEA FILE=REGISTRY SUB=L37 SSS FUL L66

100.0% PROCESSED 6577 ITERATIONS SEARCH TIME: 00.00.01

110 ANSWERS

=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 14:49:33 ON 10 DEC 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d 180 1-18 cbib abs hitstr hitind

L80 ANSWER / OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
2004:722950 Document No. 141:244924 Dye compounds exhibiting
different colors in crystalline form and in liquid form and their use

imaging members and imaging method. Allen, Richard M.;
Filosa, Michael P.; Telfer, Stephen J. (USA). U.S. Pat. Appl. Publ.

2004171817 A1 20040902, 9 pp. (English). CODEN: USXXCO.

APPLICATION: US

2004-789600 20040227. PRIORITY: US 2003-PV451208 20030228.

GΙ

US

AB The dye compound I (R1-5, R7 = H, (un) substituted alkyl, (un) substituted alkenyl, (un) substituted alkynyl, (un) substituted heterocycloalkyl, substituted carbonyl, acylamino, halogen, nitro,

<WALKE 10/789566><Page 12>

nitrilo, sulfonyl, aryl, substituted aryl, (un) substituted heteroaryl, (un) substituted oxygen, (un) substituted nitrogen, and (un) substituted sulfur; R6 = halogen, (un) substituted oxygen, (un) substituted nitrogen and (un) substituted sulfur; R8-11 = H, (un) substituted alkyl, (un) substituted alkenyl, (un) substituted alkynyl, (un) substituted heterocycloalkyl, substituted carbonyl, acylamino, halogen, nitro, nitrilo, sulfonyl, aryl, substituted aryl, (un) substituted heteroaryl, (un) substituted oxygen, (un) substituted nitrogen and (un) substituted sulfur; X1 = carbonyl, methylene, substituted methylene and sulfonyl; X2 = oxygen, (un) substituted nitrogen; X3 = oxygen, sulfur and (un) substituted nitrogen; X4 = carbon, nitrogen; and A = hydrogen-bond accepting group) are formed between hydrogen bond acceptors and phenolic dye The imaging method comprises (a) providing an imaging member comprising a first image-forming layer including the dye compound in the crystalline form; and (b) converting at least а portion of the compound to the liquid form in an imagewise pattern whereby an image is formed. ΙΤ 748802-87-1 748802-89-3 748802-91-7 748802-93-9 748802-95-1 748802-97-3 748802-99-5 748803-01-2 748803-03-4 RL: TEM (Technical or engineered material use); USES (Uses) (dye compds. exhibiting different colors in crystalline form and in liquid form for imaging members) 748802-87-1 HCAPLUS RN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3'-hydroxy-6'-CN (phenylmethoxy) -, compd. with 1,10-phenanthroline (1:1) (9CI) (CA INDEX NAME) CM 1 327594-34-3 CRN CMF C27 H18 O5

<WALKE 10/789566><Page 13>

CM 2

CRN 66-71-7 CMF C12 H8 N2

RN 748802-89-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3'-hydroxy-6'(phenylmethoxy)-, compd. with 2,9-dimethyl-1,10-phenanthroline (1:1)
(9CI)

(CA INDEX NAME)

CM 1

CM 2

CRN 484-11-7 CMF C14 H12 N2

RN 748802-91-7 HCAPLUS

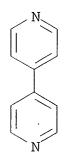
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3'-hydroxy-6'(phenylmethoxy)-, compd. with 4,4'-bipyridine (2:1) (9CI) (CA INDEX NAME)

CM 1

<WALKE 10/789566><Page 15>

CM 2

CRN 553-26-4 CMF C10 H8 N2



CN

RN 748802-93-9 HCAPLUS

Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3'-hydroxy-6'-(phenylmethoxy)-, compd. with pyrazine (1:1) (9CI) (CA INDEX NAME)

CM 1

CM 2

CRN 290-37-9 CMF C4 H4 N2



RN 748802-95-1 HCAPLUS

CN 2-Pyridinecarboxylic acid, ethyl ester, compd. with 3'-hydroxy-6'- (phenylmethoxy)spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one (1:1) (9CI)

(CA INDEX NAME)

CM 1

<WALKE 10/789566><Page 17>

CM 2

CRN 2524-52-9 CMF C8 H9 N O2

RN 748802-97-3 HCAPLUS

CN Spiro[isobenzofuran-1,9'-[9H]xanthen]-3-one,

2',7'-diethyl-3'-hydroxy-6'-

(phenylmethoxy)-, compd. with 4,4'-bipyridine (2:1) (9CI) (CA INDEX

NAME)

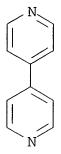
CM 1

CRN 748802-96-2 CMF C31 H26 O5

CM 2

CRN 553-26-4

CMF C10 H8 N2



RN 748802-99-5 HCAPLUS
CN Spiro[isobenzofuran-1,9'-[9H]xanthen]-3-one,
3'-ethoxy-2',7'-dihexyl-6'hydroxy-, compd. with 4,4'-bipyridine (2:1) (9CI) (CA INDEX NAME)

CM 1

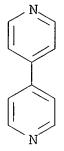
CRN 748802-98-4 CMF C34 H40 O5

Me-
$$(CH_2)_5$$
OEt

(CH₂)₅-Me

CM 2

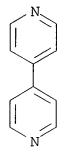
CRN 553-26-4 CMF C10 H8 N2



CM 2

CRN 553-26-4

CMF C10 H8 N2



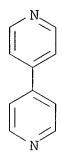
RN 748803-03-4 HCAPLUS
CN Spiro[isobenzofuran-1,9'-[9H]xanthen]-3-one,
3'-hydroxy-6'-(phenylmethoxy)2',7'-bis(phenylmethyl)-, compd. with 4,4'-bipyridine (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 748803-02-3 CMF C41 H30 O5

CM 2

CRN 553-26-4 CMF C10 H8 N2



```
IC
     ICM C09B056-00
         G03C005-18
NCL
     534653000; 156235000; 430151000
     41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and
CC
Photographic
     Sensitizers)
     hydrogen bond acceptor phenolic dye compd; color different cryst
ST
     lig form imaging
IT
     Imaging
       Optical imaging devices
        (dye compds. exhibiting different colors in crystalline form and
        in liquid form for imaging members)
ΙT
     Dyes
        (dye complexes exhibiting different colors in crystalline form and
        in liquid form and their use in imaging members and
        imaging method)
     748802-87-1 748802-89-3 748802-91-7
IT
     748802-93-9 748802-95-1 748802-97-3
     748802-99-5 748803-01-2 748803-03-4
     748803-05-6
                   748803-07-8
                                 748803-09-0
                                               748803-11-4
                                                             748803-13-6
     748803-15-8
                   748803-17-0
                                 748803-19-2
                                               748803-21-6
                                                             748803-23-8
     748803-25-0
                   748803-26-1
                                748803-27-2
                                               748803-28-3
                                                             748803-29-4
     748803-30-7
                  748803-31-8
                                 748803-32-9
                                               748803-33-0
                                                             748803-34-1
     748803-35-2
                   748803-36-3
                                748803-37-4
                                               748803-38-5
                                                             748803-39-6
     748803-40-9
     RL: TEM (Technical or engineered material use); USES (Uses)
```

L80 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN 2004:502261 Document No. 141:98470 Fluorescent pH sensors with negligible

in liquid form for imaging members)

sensitivity to ionic strength. Weidgans, Bernhard M.; Krause, Christian;

Klimant, Ingo; Wolfbeis, Otto S. (Institute of Analytical Chemistry, Chemo- and Biosensors, University of Regensburg, Regensburg, D-93040,

(dye compds. exhibiting different colors in crystalline form and

<WALKE 10/789566><Page 22>

Germany). Analyst (Cambridge, United Kingdom), 129(7), 645-650 (English)

2004. CODEN: ANALAO. ISSN: 0003-2654. Publisher: Royal Society of Chemistry.

AB Optical pH determination has the fundamental disadvantage of measuring a

signal that depends on the ionic strength of the sample. The problem originates from the complex relation between the proton activity and the

concentration of the pH-sensitive $\ensuremath{\mbox{dye}}$. The effect of ionic strength on

the signal depends on the charge of the indicator and its environment, e.g. the immobilization matrix. The authors present novel lipophilic fluorescein esters carrying one neg. charge. They are embedded in an uncharged, highly proton-permeable hydrogel to give optical pH sensors that show a negligible cross-sensitivity towards ionic strength.

The fluorescent **dyes** differ in their substituents. This variation of substituents results in dissociation consts. between 5.5 and 8.5.

The indicators were made lipophilic by esterification of the carboxy group

with a C18 alkyl chain. Since their spectral properties are quite similar, two indicators may be used in one sensor. This results in an optical pH sensor with a dynamic range that extends from pH 4.5 to 8.

IT 124119-87-5 714951-32-3

RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)

(fluorescent pH sensors with negligible sensitivity to ionic strength $% \left(1\right) =\left(1\right) +\left(1$

based on fluorescent dyes)

RN 124119-87-5 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',7'-dihexyl-3',6'-dihydroxy-(9CI) (CA INDEX NAME)

RN 714951-32-3 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,
2'-chloro-7'-hexyl-3',6'dihydroxy- (9CI) (CA INDEX NAME)

CC 79-2 (Inorganic Analytical Chemistry)

IT Ionic strength

Optical sensors

Нq

(fluorescent pH sensors with negligible sensitivity to ionic strength)

IT Fluorescent dyes

(fluorescent pH sensors with negligible sensitivity to ionic strength $\ensuremath{\mathcal{C}}$

based on fluorescent dyes)

IT 76-54-0 2321-03-1 **124119-87-5 714951-32-3**

714951-33-4 714951-34-5 714951-35-6 714951-36-7 714951-37-8 RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)

(fluorescent pH sensors with negligible sensitivity to ionic strength $\ensuremath{\mathcal{C}}$

based on fluorescent dyes)

L80 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

2004:351274 Document No. 140:357221 High purity phthaleines and their preparation process using an organic ester as cyclocondensation solvent

and a strong acid to precipitate them. Tran, Guyon Joanne; Scherninski,

Francois (Laboratoires Synth-Innove, Fr.). Fr. Demande FR 2846331 Al 20040430, 41 pp. (French). CODEN: FRXXBL. APPLICATION: FR 2002-13528

20021029.

GΙ

<WALKE 10/789566><Page 24>

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is related to the preparation of high purity phthaleines I (< 1% $\,$

in weight, especially < 0.2% in weight impurities), in particular fluoresceines, by

cyclocondensation of phthalic anhydride is with a naphthol or phenol in an

organic ester and in-situ acidulation of the crystalline product with a strong

acid. These high purity phthaleines are useful for medical imaging and in the field of biotechnol. For example, condensation of phthalic anhydride with resorcinol in Me benzoate at 200° for 6 h gave 78% red crystals of crude fluoresceine (II), which was dissolved in

EtOH/acetone, acidulated with concentrated H2SO4, to give 99.8% purity II after

washing the yellow crystals with EtOH/acetone/H2O. Simillarly, 4',5'-dimethylfluoresceine and 4',5'-dihydroxyfluoreceine were prepared in

high purity.

IT 118797-71-0P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(phthalein product; preparation of high purity phthaleines using an organic

ester as cyclocondensation solvent and a strong acid to precipitate them)

RN 118797-71-0 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3',6'-dihydroxy-4',5'-

dimethyl- (9CI) (CA INDEX NAME)

```
IC
     ICM C07D493-10
          A61K031-353; A61K049-00; C07D311-00; C07D307-00
     27-20 (Heterocyclic Compounds (One Hetero Atom))
CC
     Section cross-reference(s): 1, 9, 41, 45
     2103-64-2P 118797-71-0P
ΙT
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (phthalein product; preparation of high purity phthaleines using
an organic
        ester as cyclocondensation solvent and a strong acid to
precipitate them)
L80 ANSWER 4 OF 18 HCAPLUS
                              COPYRIGHT 2004 ACS on STN
2004:143027 Document No. 140:201792 Color-coded layer-by-layer
microcapsules
     serving as combinatorial analysis libraries and as specific
     optical sensors. Daehne, Lars; Baude, Barbara; Voigt, Andreas
     (Capsulution Nanoscience Ag, Germany). PCT Int. Appl. WO 2004014540
Α1
     20040219, 39 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ,
BA,
     BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC,
EE,
     ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP,
KR,
     KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI,
NO,
     NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
TN,
     TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF,
BJ,
     CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU,
MC,
     ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (German). CODEN: PIXXD2.
     APPLICATION: WO 2003-EP8376 20030729. PRIORITY: DE 2002-10236409
     20020802; DE 2003-10315846 20030402.
AB
     Capsules are described which have diams. of <100 \mu m and which are
     coated with ≥3 polyelectrolyte layers, ≥1 of the layers
     being marked with a dye. Different fluorescent dyes
     may be covalently bound in a defined amount to the polyelectrolytes.
The
     amount of dye may be controlled by varying the label content or by
     the codeposition of unlabeled polymers. Different dye layers
     may be separated from one another by intermediate layers thereby
suppressing
     unwanted interactions. Alternately, a fluorescence resonant energy
```

transfer (FRET) signal may be generated between suitable dye

<WALKE 10/789566><Page 26>

pairs situated at short distances (0-6 nm) from one another. This signal

may be controlled independently of the **dye** concentration by the number of

intermediate layers. The capsule coding may be read out by the variation

in the excitation wavelength and emission wavelength. Macromols. may be

immobilized inside the capsules and extract complementary substances out of

solns. Particles coated in such a manner or hollow capsules may be used

as sensors after inserting a sensitive intermediate layer. Changes in the

size/structure of the intermediate layer may be detected either by $\ensuremath{\mathsf{FRET}}$

between adjacent, labeled polyelectrolyte layers or by the self-quenching/aggregate fluorescence of **dyes** in the sensitive layer. Systems for identifying or marking materials comprising ≥ 2 of types of capsules are also described.

IT 661466-06-4

RL: ARU (Analytical role, unclassified); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)

(color-coded layer-by-layer microcapsules useful as combinatorial anal.

libraries and as specific optical markers)

RN 661466-06-4 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

ar-isothiocyanato-3',6'-

dihydroxy-2',7'-dimethyl- (9CI) (CA INDEX NAME)

D1-N=C=S

IC ICM B01J013-02

ICS B01J013-22

CC 48-11 (Unit Operations and Processes)

Section cross-reference(s): 9, 63, 79, 80

IT Acid-base indicators

Colorimetric indicators

Combinatorial library

Fluorescent indicators

Polyelectrolytes

(color-coded layer-by-layer microcapsules useful as combinatorial anal.

libraries and as specific optical markers)

IT Capsules

ZP4,

(color-coded; color-coded layer-by-layer microcapsules useful as combinatorial anal. libraries and as specific **optical** markers)

IT 50851-57-5 71550-12-4, Poly(allylamine hydrochloride) 661465-58-3 661466-06-4 661466-07-5

RL: ARU (Analytical role, unclassified); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)

(color-coded layer-by-layer microcapsules useful as combinatorial anal.

libraries and as specific optical markers)

L80 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN 2003:49660 Document No. 138:250988 ZP4, an improved neuronal Zn2+sensor of

the zinpyr family. Burdette, Shawn C.; Frederickson, Christopher J.; Bu,

Weiming; Lippard, Stephen J. (Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA). Journal of the American Chemical Society, 125(7), 1778-1787 (English) 2003. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB A second-generation fluorescent sensor for Zn2+ from the Zinpyr family,

ZP4, has been synthesized and characterized. ZP4 (Zinpyr-4, 9-(o-carboxyphenyl)-2-chloro-5-[2-{bis(2-pyridylmethyl)aminomethyl}-N-methylaniline]-6-hydroxy-3-xanthanone) is prepared via a convergent synthetic strategy developed from previous studies with these compds.

like its predecessors, has excitation and emission wavelengths in the visible range (.apprx.500 nm), a dissociation constant (Kd) for Zn2+ of less

than 1 nM and a high quantum yields (Φ = .apprx.0.4), making it well suited for biol. applications. A 5-fold fluorescent enhancement is observed

under simulated physiol. conditions corresponding to the binding of the

Zn2+ cation to the sensor, which inhibits a photoinduced electron transfer

```
(PET) quenching pathway. The metal-binding stereochem. of ZP4 was
     evaluated through the synthesis and x-ray structural characterization
of
     [M(BPAMP)(H2O)n] + complexes, where BPAMP is [2-{bis(2-
     pyridylmethyl) aminomethyl}-N-methylaniline|-phenol and M = Mn2+, Zn2+
(n =
     1) or Cu2+(n = 0).
ΙT
     389625-48-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); .
RACT
     (Reactant or reagent)
        (ZP4, an improved neuronal Zn2+ sensor of zinpyr family)
RN
     389625-48-3
                 HCAPLUS
     Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,
2'-chloro-3',6'-dihydroxy-
     5'-methyl- (9CI) (CA INDEX NAME)
```

```
9-14 (Biochemical Methods)
CC
ΙΤ
     Imaging
        (fluorescent; ZP4, an improved neuronal Zn2+ sensor of zinpyr
family)
     2513-23-7P 389625-48-3P
                               389625-49-4P
                                              389625-50-7P
ΤТ
     502467-15-4P
                    502467-17-6P
                                   502467-19-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (ZP4, an improved neuronal Zn2+ sensor of zinpyr family)
     ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
L80
              Document No. 139:97443 Production, characteristics and
     applications of fluorescent PEBBLE nanosensors: potassium, oxygen,
calcium
     and pH imaging inside live cells. Brasuel, Murphy; Kopelman,
     Raoul; Aylott, Jonathan W.; Clark, Heather; Xu, Hao; Hoyer, Marion;
```

<WALKE 10/789566><Page 29>

Miller, Terry J.; Tjalkens, Ron; Philbert, Martin A. (Department of Chemistry, The University of Michigan, Ann Arbor, MI, 48109, USA). Sensors and Materials, 14(6), 309-338 (English) 2002. CODEN: SENMER. ISSN: 0914-4935. Publisher: Scientific Publishing Division of MYU K.K..

AB A novel platform for the intracellular monitoring of key biol. components

has been developed, using three different nanoparticle fabrication technologies. These nano-optodes are termed PEBBLEs (Probes Encapsulated

By Biol. Localized Embedding). The sensors, based on polyacrylamide, cross-linked decyl methacrylate, and silica-based sol-gel, have been characterized in aqueous solution and also tested in intracellular surroundings.

Each matrix can be combined with specific "free dyes", ionophores, or enzymes to produce sensors selective for the biol. component of interest. Spherical sensors less than 600 nm in diameter (and

reducible to below 100 nm) have been made from all three matrixes. Acrylamide-based sensors have been used to monitor intracellular pH and

calcium (with proven selectivity over Mg2+). Decyl methacrylate has been

successfully applied to intracellular potassium monitoring with probes 1,000 times more selective for potassium than sodium. Sol-gel has proven

useful for monitoring intracellular oxygen at physiol. interesting concns.

PEBBLEs, with a wide range of both simple and complex sensing schemes, provide a unique tool for minimally invasive intracellular monitoring, with many significant advantages over free dyes as well as over fiber-optic sensors.

IT 100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein
100111-03-3, 6-Carboxy-4',5'-dimethylfluorescein
RL: ARG (Analytical reagent use); DEV (Device component use); ANST
(Analytical study); USES (Uses)

(entrapped fluorescent pH sensitive dye; production, characterization and applications of PEBBLE nanooptrodes containing entrapped fluorescent probes for potassium, oxygen, calcium and pH imaging inside live cells)

RN 100111-02-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

RN 100111-03-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

CC 9-1 (Biochemical Methods)

IT Biosensors

Optrodes

(fluorescent, PEBBLE (Probes Encapsulated By Biol. Localized Embedding); production, characterization and applications of PEBBLE nanooptrodes containing entrapped fluorescent probes for potassium, oxygen,

calcium and pH imaging inside live cells)

IT Polyoxyalkylenes, uses

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(in sol-gel PEBBLE; production, characterization and applications of PEBBLE

nanooptrodes containing entrapped fluorescent probes for potassium, oxygen,

calcium and pH imaging inside live cells)

```
IT
     Animal cell
     Fluorescent indicators
     Fluorometry
     Hq
        (production, characterization and applications of PEBBLE
nanooptrodes
        containing entrapped fluorescent probes for potassium, oxygen,
calcium and
        pH imaging inside live cells)
     100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein
ΙT
     100111-03-3, 6-Carboxy-4',5'-dimethylfluorescein
                                                         131071-70-0
     131084-60-1
                   132234-44-7, ETH5350
                                          145103-60-2, 5-
                                 145103-61-3, 6-Carboxynaphthofluorescein
     Carboxynaphthofluorescein
     202872-98-8
                  445289-99-6
     RL: ARG (Analytical reagent use); DEV (Device component use); ANST
     (Analytical study); USES (Uses)
        (entrapped fluorescent pH sensitive dye; production,
        characterization and applications of PEBBLE nanooptrodes containing
        entrapped fluorescent probes for potassium, oxygen, calcium and pH
        imaging inside live cells)
ΙT
     99348-39-7, BME-44
     RL: ARG (Analytical reagent use); DEV (Device component use); ANST
     (Analytical study); USES (Uses)
        (entrapped fluorescent potassium probe; production,
characterization and
        applications of PEBBLE nanooptrodes containing entrapped
fluorescent probes
        for potassium, oxygen, calcium and pH imaging inside live
        cells)
ΙT
     138067-55-7, Calcium green 138067-56-8, Calcium orange
     RL: ARG (Analytical reagent use); DEV (Device component use); ANST
     (Analytical study); USES (Uses)
        (entrapped fluorescent probe; production, characterization and
applications
        of PEBBLE nanooptrodes containing entrapped fluorescent probes for
        potassium, oxygen, calcium and pH imaging inside live cells)
ΙT
     60311-02-6, Sulforhodamine 101
     RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
     (Uses)
        (entrapped fluorescent reference probe; production,
characterization and
        applications of PEBBLE nanooptrodes containing entrapped
fluorescent probes
        for potassium, oxygen, calcium and pH imaging inside live
        cells)
     105560-52-9
IT
     RL: BUU (Biological use, unclassified); DEV (Device component use);
BIOL
```

```
(Biological study); USES (Uses)
        (entrapped, ionic additive; production, characterization and
applications
        of PEBBLE nanooptrodes containing entrapped fluorescent probes for
        potassium, oxygen, calcium and pH imaging inside live cells)
     122-62-3, Dioctyl sebacate 3179-47-3, Decyl methacrylate
ΙΤ
58264-26-9,
     Hexanedioldimethacrylate
     RL: ARU (Analytical role, unclassified); DEV (Device component use);
ANST
     (Analytical study); USES (Uses)
        (in decyl methacrylate PEBBLE nanosensor; production,
characterization and
        applications of PEBBLE nanooptrodes containing entrapped
fluorescent probes
        for potassium, oxygen, calcium and pH imaging inside live
        cells)
                9003-05-8, PolyAcrylamide
IT
     110-26-9
     RL: ARU (Analytical role, unclassified); DEV (Device component use);
ANST
     (Analytical study); USES (Uses)
        (in polyacrylamide PEBBLE nanosensor; production, characterization
and
        applications of PEBBLE nanooptrodes containing entrapped
fluorescent probes
        for potassium, oxygen, calcium and pH imaging inside live
     9004-54-0D, Dextran, conjugate with Oregon Green 488
ΙT
                                                             195136-58-4D,
     Oregon Green 488, dextran conjugate
     RL: ARG (Analytical reagent use); DEV (Device component use); ANST
     (Analytical study); USES (Uses)
        (in sol-gel PEBBLE; production, characterization and applications
of PEBBLE
        nanooptrodes containing entrapped fluorescent probes for
potassium, oxygen,
        calcium and pH imaging inside live cells)
     25322-68-3, Polyethylene glycol
IT
     RL: DEV (Device component use); TEM (Technical or engineered material
     use); USES (Uses)
        (in sol-gel PEBBLE; production, characterization and applications
of PEBBLE
        nanooptrodes containing entrapped fluorescent probes for
potassium, oxygen,
        calcium and pH imaging inside live cells)
ΙT
     36309-88-3
     RL: ARG (Analytical reagent use); DEV (Device component use); ANST
     (Analytical study); USES (Uses)
        (indicator dye in sol-gel PEBBLE; production, characterization
```

<WALKE 10/789566><Page 33>

and applications of PEBBLE nanooptrodes containing entrapped fluorescent

probes for potassium, oxygen, calcium and pH imaging inside live cells)

IT 7440-09-7, Potassium, analysis 7440-70-2, Calcium, analysis 7782-44-7,

Oxygen, analysis

RL: ANT (Analyte); ANST (Analytical study)

(production, characterization and applications of PEBBLE nanooptrodes

containing entrapped fluorescent probes for potassium, oxygen, calcium and

pH imaging inside live cells)

IT 78-10-4, Tetraethyl orthosilicate

RL: CAT (Catalyst use); USES (Uses)

(production, characterization and applications of PEBBLE nanooptrodes

containing entrapped fluorescent probes for potassium, oxygen, calcium and

pH imaging inside live cells)

L80 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN 2002:707363 Document No. 137:249241 Ink-jet recording inks and their use in

the manufacture of color filters for liquid-crystal display panels. Hirose, Masashi (Canon Inc., Japan). Jpn. Kokai Tokkyo Koho JP 2002265834

A2 20020918, 19 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2001-74329 20010315.

AB The inks with good transparency and adhesion to substrate surface, contain

azo pyridone **dye** of R1N:NR2 (I) type (R1 = Ph groups optionally substituted with halogen, OH, CN, NO2, amino, phosphonyl, sulfonyl, sulfamido group, etc.; R2 = 6-hydroxypyridon-5-yl group optionally substituted with alkyl, COOH, CF3 group on position 4, with CN, carbamoyl,

sulfonyl, methylsulfonyl group or their salt on position 3 and with alkyl,

polysulfonated group or their salt), xanthene-type **dyes** and water-soluble organic solvents. The inks are used as a red ink of multiple

color inks in the printing of a transparent color filter substrate bearing

an ink receiving layer. Thus, a red ink was prepared from I (R1 = 3-NaO3SC6H4; R2 = 1-butyl-3-carbamoyl-4-methyl-6-hydroxypyridon-5-yl group) 3, C.I.Acid Red 52 (xanthene-type pigment) 3, ethylene glycol monobutyl ether 39, EtOH 6 and water 49%.

IT 460352-22-1D, sodium salt

Na

IC ICM C09D011-00 ICS B41J002-01; C09B067-22; C09B067-46; G02B005-20; G02F001-1335; C09B011-28; C09B029-42

CC 42-12 (Coatings, Inks, and Related Products) Section cross-reference(s): 74, 76

ST optical color filter LCD manuf ink jet ink pigment; xanthene azopyridone red pigment color filter manuf jet ink

IT Azo dyes

Ink-jet printing

Liquid crystal displays

Optical filters

(ink-jet recording inks and use in manufacture of color filters for liquid-crystal display panels)

IT Dyes

(xanthene; ink-jet recording inks and use in manufacture of color filters

for liquid-crystal display panels)

<WALKE 10/789566><Page 35>

- IT 3520-42-1, C.I.Acid Red 52 12220-28-9, C.I.Acid Red 289 366806-34-0
 - 366806-35-1 366806-36-2 366806-37-3 366806-38-4 **460352-22-1D** , sodium salt
- RL: TEM (Technical or engineered material use); USES (Uses) (pigment; ink-jet recording inks and use in manufacture of color filters for
 - liquid-crystal display panels)
- L80 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN 2000:67416 Document No. 132:87481 Aerosol-generated sol-gel derived thin
- films and applications thereof. Bright, Frank V.; Colon, Luis A.; Jordan,
- Jeffrey D.; Dunbar, Richard A. (Research Foundation of Suny At Buffalo,
 - USA). U.S. US 6016689 A 20000125, 22 pp. (English). CODEN: USXXAM. APPLICATION: US 1996-752460 19961118.
- AB A sensor having a substrate overlayed with a sol-gel layer, a chemical sensing species deposited upon the sol-gel layer, and a thin film of a 2nd
- sol-gel layer overlaying and entrapping the species. The effect of this
- sensor is that the species exhibits a significant portion of its intrinsic
- function over a period of time. In yet another embodiment of the subject
- invention, a method is disclosed to form a thin sol-gel layer upon an ambient substrate. This method ensures the integrity, stability and functionality of the chemical sensing species within the sol-gel layers.
- IT 100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein 100111-03-3, 6-Carboxy-4',5'-dimethylfluorescein
 - RL: ANT (Analyte); ANST (Analytical study)
 - (carboxy di-Me fluorescein determination in solution **optical** sensor based on fluorescence using sol-gel immobilized antibody as sensing element)
- RN 100111-02-2 HCAPLUS
- CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

RN 100111-03-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo- (9CI) (CA INDEX NAME)

IC ICM G01N007-00

NCL 073031050

CC 80-2 (Organic Analytical Chemistry)

Section cross-reference(s): 9

IT Immobilization, biochemical

(antibody; carboxy di-Me fluorescein determination in solution optical

sensor based on fluorescence using sol-gel immobilized antibody as sensing element)

IT Fluorescence

Optical sensors

(carboxy di-Me fluorescein determination in solution **optical** sensor based on fluorescence using sol-gel immobilized antibody as sensing element)

IT Antibodies

RL: ARG (Analytical reagent use); DEV (Device component use); ANST

(Analytical study); USES (Uses)

(immobilized; carboxy di-Me fluorescein determination in solution optical

sensor based on fluorescence using sol-gel immobilized antibody as sensing element)

IT 100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein 100111-03-3, 6-Carboxy-4',5'-dimethylfluorescein

RL: ANT (Analyte); ANST (Analytical study)
(carboxy di-Me fluorescein determination in solution optical sensor based on fluorescence using sol-gel immobilized antibody as sensing element)

L80 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

1999:624082 Document No. 132:32735 Optical Nanosensors for Chemical Analysis inside Single Living Cells. 2. Sensors for pH and Calcium and the Intracellular Application of PEBBLE Sensors. Clark, Heather A.; Kopelman, Raoul; Tjalkens, Ron; Philbert, Martin A. (Department of Chemistry and Department of Environmental Health Sciences,

University of Michigan, Ann Arbor, MI, 48109-1055, USA). Analytical Chemistry, 71(21), 4837-4843 (English) 1999. CODEN: ANCHAM. ISSN: 0003-2700. Publisher: American Chemical Society.

AB Optical nanosensors, or PEBBLEs (probes encapsulated by biol. localized embedding), have been produced for intracellular measurements of

pH and calcium. Five varieties of pH-sensitive sensors and three different calcium-selective sensors are presented and discussed. Each sensor combines an ion-selective fluorescent indicator and an ion-insensitive internal standard entrapped within an acrylamide polymeric

matrix. Calibrations and linear ranges are presented for each sensor. The photobleaching of **dyes** incorporated into PEBBLEs is comparable to that of the resp. free **dye** that is incorporated within the matrix. These PEBBLE sensors are fully reversible over

many $$\operatorname{\textsc{measurements}}$.$ The leaching of fluorescent indicator from the polymer is

less than 50% over a 48-h period (note that a typical application time is

only a few hours). The PEBBLE sensors have also been applied to intracellular anal. of the calcium flux in the cytoplasm of neural cells

during the mitochondrial permeability transition. Specifically, a distinct

difference is noted between cells of different types (astrocyte vs neuron-derived cells) with respect to their response to the toxicant m-dinitrobenzene (DNB). Use of PEBBLE sensors permits the quant. discrimination of subtle differences between the ability of human SY5Y

neuroblastoma and C6 glioma to respond to challenge with DNB. Specifically, measurement of intracellular calcium, the precursor to cell

death, has been achieved.

IT 103991-76-0

RL: ARU (Analytical role, unclassified); ANST (Analytical study) (optical nanosensors for chemical anal. inside single living cells and sensors for pH and calcium and the intracellular application

of PEBBLE sensors)

RN 103991-76-0 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-ar-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo- (9CI) (CA INDEX NAME)

D1-CO2H

CC 9-1 (Biochemical Methods)

ST optical PEBBLE sensor cell pH calcium

IT Neuroglia

(glioma; optical nanosensors for chemical anal. inside single living cells and sensors for pH and calcium and the intracellular application of PEBBLE sensors)

IT Nerve, neoplasm

(neuroblastoma; optical nanosensors for chemical anal. inside single living cells and sensors for pH and calcium and the intracellular application of PEBBLE sensors)

IT Biosensors

Cell

Cytoplasm

Fluorescent dyes

Hq

(optical nanosensors for chemical anal. inside single living

<WALKE 10/789566><Page 39>

cells and sensors for pH and calcium and the intracellular application of PEBBLE sensors)

IT Polymers, uses

RL: DEV (Device component use); USES (Uses)

(optical nanosensors for chemical anal. inside single living cells and sensors for pH and calcium and the intracellular application

of PEBBLE sensors)

IT 99-65-0, m-Dinitrobenzene

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (optical nanosensors for chemical anal. inside single living cells, and sensors for pH and calcium and the intracellular application

of PEBBLE sensors)

IT 7440-70-2, Calcium, analysis

RL: ANT (Analyte); ANST (Analytical study)

(optical nanosensors for chemical anal. inside single living cells and sensors for pH and calcium and the intracellular application

of PEBBLE sensors)

IT 60311-02-6, Sulforhodamine 101 **103991-76-0** 128724-35-6 131071-60-8, SNAFL-1 138067-55-7, Calcium green 138067-56-8, Calcium

orange 153130-66-6, Calcium green 5N 155898-75-2 252321-13-4 RL: ARU (Analytical role, unclassified); ANST (Analytical study) (optical nanosensors for chemical anal. inside single living cells and sensors for pH and calcium and the intracellular application

of PEBBLE sensors)

L80 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
1997:424380 Document No. 127:146558 Photon-counting optical-fiber
sensor for the detection of ammonia in neurochemical applications.
Elamari, A.; Gisin, N.; Munoz, J. L.; Poitry, S.; Tsacopoulos, M.;
Zbinden, H. (University of Geneva, Group of Applied Physics, 20,

ecole de

Medecine CH-1211, Geneva, 4, Switz.). Sensors and Actuators, B: Chemical,

B38(1-3), 183-188 (English) 1997. CODEN: SABCEB. ISSN: 0925-4005. Publisher: Elsevier.

AB We report our progress in developing a miniaturized version of an optical-fiber sensor for the measurement of ammonia. The principle of the measurement is based on the combination of photon counting and fluorescence from a pH indicator. This sensor has been developed to monitor the release of ammonia by photoreceptors of the honeybee drone retina under stimulation by light or by a chemical It has a

<WALKE 10/789566><Page 40>

dynamic of 25 dB and a detection limit of 30 nM. Sensors for other chems.

could be constructed on the same principle, by simply changing the indicator used.

IT 100111-02-2

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (photon-counting optical-fiber sensor for ammonia detection in neurochem. studies)

RN 100111-02-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

CC 9-1 (Biochemical Methods)

Section cross-reference(s): 13, 73, 79

ST ammonia detection optical fiber sensor; photon counting fiber optic sensor ammonia; honeybee photoreceptor ammonia release detection

IT Optical detectors

(fluorescence; photon-counting optical-fiber sensor for ammonia detection in neurochem. studies)

IT Honeybee

(photon-counting optical-fiber sensor for ammonia detection in neurochem. studies)

IT Fiber optic sensors

(photon-counting; photon-counting optical-fiber sensor for ammonia detection in neurochem. studies)

IT Eye Eve

(photoreceptor; photon-counting optical-fiber sensor for ammonia detection in neurochem. studies)

IT 7664-41-7, Ammonia, analysis 14798-03-9, Ammonium, analysis RL: ANT (Analyte); ANST (Analytical study) (photon-counting optical-fiber sensor for ammonia detection

in neurochem. studies)

IT 100111-02-2

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (photon-counting optical-fiber sensor for ammonia detection in neurochem. studies)

L80 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN 1996:42936 Document No. 124:163654 Optical sensor system for determining pH values and ionic strengths. Alder, Alex; Barnard, Steven;

Berger, Joseph; Blom, Nils; Rouilly, Marizel (Ciba-Geigy A.-G., Switz.).

PCT Int. Appl. WO 9530148 A1 19951109, 50 pp. DESIGNATED STATES: W: AM,

AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ,

LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM,

TT, UA, US, UZ, VN; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES,

FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1995-IB302 19950427. PRIORITY: CH 1994-1360 19940502.

AB A method for the independent, reversible, optical determination of pH value and th ionic strength of an aqueous sample with the aid of two different

sensors in accordance with the fluorescence method, in which method two

optical sensors, which are each composed of polymers of different structure but each contains the same fluorescent dye and which each consists of a coated material composed of (a) a carrier material, to

which there applied (b) at least one water-insol. layer of a polymer comprising at least one hydrophilic monomer (A) from the group of substituted olefins, and (c) a proton-sensitive fluorescent dye which is bonded directly or via a bridge group to the spine of polymer (b)

or which is incorporated in polymer (b), are brought into contact with an

aqueous test sample, irradiated with exciting light, the fluorescence is

measured and the pH values and the ionic strengths are calculated from the

measured fluorescence intensities with reference to calibration curves.

IT 172530-91-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(a NH-optical sensor system for determining pH values and ionic strengths of aqueous samples based on two sensors containing polymers with

<WALKE 10/789566><Page 42>

different structures and same fluorescent dye)

RN 172530-91-5 HCAPLUS

CN 2-Propenamide, N-(3',6'-dihydroxy-2',4',5',7'-tetramethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)- (9CI) (CA INDEX NAME)

IT 172531-31-6P 172531-32-7P 172923-56-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

different structures and same fluorescent dye)

RN 172531-31-6 HCAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one,

5-amino-3', 6'-dihydroxy-

4',5'-dimethyl- (9CI) (CA INDEX NAME)

$$H_2N$$
 Me
 Me
 Me
 OH
 OH

RN 172531-32-7 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 6-amino-3',6'-dihydroxy-4',5'-dimethyl-(9CI) (CA INDEX NAME)

RN 172923-56-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,
3',6'-dihydroxy-4',5'dimethyl-5(or 6)-nitro- (9CI) (CA INDEX NAME)

 $D1-NO_2$

IT 172530-82-4P 172530-83-5P 172530-84-6P 172530-85-7P 172530-86-8P 172530-87-9P 172530-88-0P 172530-89-1P 172530-90-4P 172530-92-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (optical sensor system for determining pH values and ionic strengths of aqueous samples based on two sensors containing polymers with

<WALKE 10/789566><Page 44>

different structures and same fluorescent dye)

RN 172530-82-4 HCAPLUS

CN 2-Propenamide,

N-(3',6'-dihydroxy-4',5'-dimethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (9CI) (CA INDEX NAME)

RN 172530-83-5 HCAPLUS

CN 2-Propenamide,

N-(3',6'-dihydroxy-4',5'-dimethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)- (9CI) (CA INDEX NAME)

RN 172530-84-6 HCAPLUS

CN 2-Propenamide,

N-(3',6'-dihydroxy-4',5'-dimethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)-2-methyl- (9CI) (CA INDEX NAME)

<WALKE 10/789566><Page 45>

RN 172530-85-7 HCAPLUS

CN 2-Propenamide,

N-(3',6'-dihydroxy-4',5'-dimethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)-2-methyl- (9CI) (CA INDEX NAME)

RN 172530-86-8 HCAPLUS

CN 2-Propenamide,

N-(3',6'-dihydroxy-2',7'-dimethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{HO} \\ \text{Me} \\ \\ \text{Me} \\ \\ \text{Me} \\ \\ \text{O} \\ \\ \text{O$$

RN 172530-87-9 HCAPLUS

CN 2-Propenamide,

N-(3',6'-dihydroxy-2',7'-dimethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)- (9CI) (CA INDEX NAME)

RN 172530-88-0 HCAPLUS

CN 2-Propenamide,

N-(3',6'-dihydroxy-2',7'-dimethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)-2-methyl- (9CI) (CA INDEX NAME)

RN 172530-89-1 HCAPLUS

CN 2-Propenamide,

N-(3',6'-dihydroxy-2',7'-dimethyl-3-oxospiro[isobenzofuran-

<WALKE 10/789566><Page 47>

1(3H),9'-[9H]xanthen]-6-yl)-2-methyl- (9CI) (CA INDEX NAME)

RN 172530-90-4 HCAPLUS

CN 2-Propenamide, N-(3',6'-dihydroxy-2',4',5',7'-tetramethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} & \text{Me} \\ \text{HO} & \text{OH} \\ \text{Me} & \text{OH} \\ \text{OH} \\ \text{OH} & \text{OH} \\ \text{OH} \\ \text{OH} & \text{OH} \\ \text{OH} \\$$

RN 172530-92-6 HCAPLUS

CN 2-Propenamide, N-(3',6'-dihydroxy-2',4',5',7'-tetramethyl-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)-2-methyl- (9CI)

(CA INDEX NAME)

IC ICM G01N031-22

ICS C08F220-54; C08F220-58; C07D311-80

CC 79-2 (Inorganic Analytical Chemistry)

Section cross-reference(s): 38, 61

ST pH ionic strength detn optical sensor

Hq

(optical sensor system for determining pH values and ionic strengths of aqueous samples based on two sensors containing polymers with

different structures and same fluorescent dye)

IT Dyes

(fluorescent, optical sensor system for determining pH values and ionic strengths of aqueous samples based on two sensors containing polymers

with different structures and same fluorescent dye)

IT Sensors

(optical, optical sensor system for determining pH values and ionic strengths of aqueous samples based on two sensors containing polymers

with different structures and same fluorescent dye)

IT Alkenes, analysis

RL: ARU (Analytical role, unclassified); DEV (Device component use); ANST

(Analytical study); USES (Uses)

with different structures and same fluorescent dye)

IT 172530-91-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(a NH-optical sensor system for determining pH values and ionic strengths of aqueous samples based on two sensors containing polymers with

<WALKE 10/789566><Page 49>

```
different structures and same fluorescent dye)
IΤ
     7732-18-5, Water, analysis
     RL: AMX (Analytical matrix); ANST (Analytical study)
        (optical sensor system for determining pH values and ionic
        strengths of aqueous samples based on two sensors containing
polymers with
        different structures and same fluorescent dve)
     110-26-9
ΤT
                868-77-9
                           7727-54-0
                                       25249-16-5
     RL: ARU (Analytical role, unclassified); DEV (Device component use);
ANST
     (Analytical study); USES (Uses)
        (optical sensor system for determining pH values and ionic
        strengths of aqueous samples based on two sensors containing
polymers with
        different structures and same fluorescent dye)
IT
     53413-37-9P
                   172531-40-7P
     RL: ARU (Analytical role, unclassified); DEV (Device component use);
SPN
     (Synthetic preparation); ANST (Analytical study); PREP (Preparation);
USES
     (Uses)
        (optical sensor system for determining pH values and ionic
        strengths of aqueous samples based on two sensors containing
polymers with
        different structures and same fluorescent dye)
ΙT
     121-44-8, reactions 530-62-1
                                      608-25-3, 2-Methylresorcinol
693-57-2,
     12-Aminododecanoic acid
                               814-68-6, Acryloyl chloride
                                                             2420-94-2,
     2-Aminoethyl methacrylate hydrochloride 3326-34-9
                                                          5197-62-6
     5292-43-3
                5466-84-2, 4-Nitrophthalic acid anhydride
                                                             20734-58-1,
     1,8-Bis(dimethylamino)naphthalene
                                         51649-83-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (optical sensor system for determining pH values and ionic
        strengths of aqueous samples based on two sensors containing
polymers with
        different structures and same fluorescent dye)
                                 172531-34-9P
ΙT
     172531-31-6P 172531-32-7P
     172923-56-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (optical sensor system for determining pH values and ionic
        strengths of aqueous samples based on two sensors containing
polymers with
        different structures and same fluorescent dye)
     45235-77-6P
IT
                   53413-38-0P
                                 72415-47-5P
                                               86520-52-7P
                                                             105502-82-7P
     172530-81-3P 172530-82-4P 172530-83-5P
     172530-84-6P 172530-85-7P 172530-86-8P
```

```
172530-87-9P 172530-88-0P 172530-89-1P
    172530-90-4P 172530-92-6P
                                 172530-93-7P
                                                172530-94-8P
    172530-95-9P
                    172530-96-0P
                                   172530-97-1P
                                                  172530-98-2P
172530-99-3P
    172531-00-9P
                    172531-01-0P
                                  172531-02-1P
                                                  172531-03-2P
172531-04-3P
    172531-05-4P
                    172531-06-5P
                                   172531-07-6P
                                                  172531-08-7P
172531-09-8P
    172531-10-1P
                    172531-11-2P
                                  172531-12-3P
                                                  172531-13-4P
172531-14-5P
                    172531-16-7P
    172531-15-6P
                                  172531-17-8P
                                                  172531-18-9P
172531-19-0P
    172531-20-3P
                    172531-21-4P
                                   172531-22-5P
                                                  172531-23-6P
172531-24-7P
                    172531-26-9P
    172531-25-8P
                                   172531-27-0P
                                                  172531-28-1P
172531-29-2P
    172531-30-5P
                    172531-33-8P
                                  172531-35-0P
                                                  172531-36-1P
172531-37-2P
    172531-38-3P
                   172531-39-4P
                                  173295-12-0P
```

RL: SPN (Synthetic preparation); PREP (Preparation)

different structures and same fluorescent dye)

IT 2530-85-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(silanizing agent; optical sensor system for determining pH values and ionic strengths of aqueous samples based on two sensors containing polymers

with different structures and same fluorescent dye)

L80 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

1995:975800 Document No. 124:134032 General model for the steady-state response properties of fiber-optic ammonia gas sensors. Li, Lin; Arnold, Mark A. (Department of Chemistry, University of Iowa, Iowa

City, IA, 52242, USA). Analytica Chimica Acta, 317(1-3), 265-73 (English)

1995. CODEN: ACACAM. ISSN: 0003-2670. Publisher: Elsevier. AB A math. model is derived to describe the steady-state response properties

of the fiber-optic ammonia sensor. Unlike the authors' previous model, the present model permits any concentration of total ammonia nitrogen

initially present in the internal solution of the sensor. A cubic equation

is solved to give the magnitude of the nonprotonated form of the indicator

<WALKE 10/789566><Page 51>

dye under equilibrium conditions. For the 1st time, the effect of the initial ammonia nitrogen concentration in the internal solution is evaluated. The

response equation is differentiated with respect to the sample ammonia concentration to give an expression that can be used to evaluate the effects of

critical exptl. parameters on the measurement sensitivity. This model is

verified by comparing predicted and actual responses for several different

fiber-optic sensor configurations. The model was used to generate surface maps that allow evaluation of the interrelationships between key exptl. parameters such as the indicator concentration, ple ammonia

concentration, internal ammonium chloride concentration and indicator acid dissociation

constant Results of this anal. indicate that optimal responses and maximal

sensitivity require careful selection of values for these parameters. 100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (as indicator for ammonia determination using fiber-optic ammonia

sensors)

ΙT

gas

RN 100111-02-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

CC 79-1 (Inorganic Analytical Chemistry)

ST modeling fiber optic ammonia gas sensor

IT Simulation and Modeling, physicochemical

(general model for steady-state response properties of fiberoptic ammonia gas sensors)

IT Sensors

<WALKE 10/789566><Page 52>

```
(gas, fiber-optic, general model for steady-state response
        properties of fiber-optic ammonia gas sensors)
     100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein
IT
     RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
        (as indicator for ammonia determination using fiber-optic ammonia
gas
        sensors)
     7664-41-7, Ammonia, analysis
ΤТ
     RL: ANT (Analyte); ANST (Analytical study)
        (general model for steady-state response properties of fiber-
        optic ammonia gas sensors)
L80 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
1995:594425 Document No. 123:73757 Sensor with improved drift stability.
     Bentsen, James G.; Wood, Kenneth B. (Minnesota Mining and
Manufacturing
     Co., USA). U.S. US 5403746 A 19950404, 44 pp.
                                                      (English). CODEN:
     USXXAM. APPLICATION: US 1993-160687 19931130.
     The present invention provides an optical fluorescence based
AB
     sensor for measuring the concentration of a gas (e.g., CO2 or
ammonia) in a
     medium such as blood which has improved drift stability.
preferred
     embodiment, the sensors of the present invention comprise
     microcompartments of an aqueous phase having a pH sensitive sensing
component
     within a hydrophobic barrier phase. The sensors of the present
invention
     are substantially free of partitioning species other than the analyte
of
     interest which can migrate from one phase to the other in response to
а
     change in pH in the aqueous phase and which substantially affect the
concentration
     dependent signal. In an alternative embodiment, the sensors of the
     present invention are constructed so as to retard the migration of
     partitioning species, thus reducing the initial rate of drift.
     100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein
ΙT
     100111-03-3, 6-Carboxy-4',5'-dimethylfluorescein
     RL: ARU (Analytical role, unclassified); DEV (Device component use);
ANST
     (Analytical study); USES (Uses)
        (pH sensitive indicator component of sensor with improved drift
        stability)
RN
     100111-02-2 HCAPLUS
     Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid,
CN
     3',6'-dihydroxy-4',5'-dimethyl-3-oxo- (9CI) (CA INDEX NAME)
```

RN 100111-03-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

IC ICM G01N033-50

ICS G01N031-00

NCL 436068000

CC 79-6 (Inorganic Analytical Chemistry)

Section cross-reference(s): 9

IT Blood analysis

(carbon dioxide and ammonia determination in blood by optical fluorescence sensor with improved drift stability)

IT Sensors

(fluorometric; carbon dioxide and ammonia determination in blood by optical fluorescence sensor with improved drift stability)

IT 7664-41-7, Ammonia, analysis

RL: ANT (Analyte); ANST (Analytical study)

(ammonia determination in blood by optical fluorescence sensor with improved drift stability)

IT 124-38-9, Carbon dioxide, analysis

```
RL: ANT (Analyte); ANST (Analytical study)
        (carbon dioxide determination in blood by optical fluorescence
sensor
        with improved drift stability)
                                    93-35-6, 7-Hydroxycoumarin
ΙT
     90-33-5, β-Methylumbelliferone
     596-09-8, Fluorescein diacetate 3301-79-9, 6-Carboxyfluorescein
     3348-03-6, 6-Carboxyfluorescein diacetate
                                                3548-09-2,
     9-Amino-6-chloro-2-methoxyacridine
                                         4733-50-0, 3,6-
     Dihydroxyphthalonitrile
                               6358-69-6, 8-Hydroxypyrene-1, 3, 6-trisulfonic
                          9000-07-1, Garrageenan 9000-30-0, Guar gum
     acid trisodium salt
     9002-89-5, Polyvinyl alcohol 9003-01-4, Poly(acrylic acid)
9003-05-8,
     Polyacrylamide
                      9003-09-2, Poly(vinyl methyl ether)
                                                           9003-39-8,
     Polyvinyl pyrrolidone
                             9004-32-4, Carboxymethylcellulose
                                                                9004-54-0,
                       9004-62-0, Hydroxyethylcellulose
     Dextran, analysis
                                                           9004-64-2,
     Hydroxypropyl cellulose 9004-65-3, Hydroxypropyl (methylcellulose)
     9004-67-5, Methylcellulose 9005-32-7, Alginic acid
                                                           9041-56-9,
     Hydroxybutyl(methylcellulose) 11138-66-2, Xanthan gum
                                                              25322-68-3
     25392-41-0, 4-Chloromethyl-7-hydroxycoumarin
                                                   26022-14-0,
     Poly(hydroxyethylacrylate) 26616-03-5
                                              26793-34-0,
     Polydimethylacrylamide
                             50851-57-5 61419-02-1, Naphthofluorescein
     62487-95-0, Poly(hydroxymethylacrylate)
                                             76823-03-5,
5-Carboxyfluorescein
     77084-71-0, Naphthofluorescein diacetate 79955-27-4,
     5-Carboxyfluorescein diacetate 100111-02-2, 5-Carboxy-4',5'-
     dimethylfluorescein 100111-03-3, 6-Carboxy-4',5'-
                          100111-04-4, 5-Carboxy-4',5'-dimethylfluorescein
     dimethylfluorescein
    diacetate
                 100111-05-5, 6-Carboxy-4',5'-dimethylfluorescein diacetate
     124412-00-6
                   126829-34-3,
2',7'-Bis-(2-carboxyethyl)-5-carboxyfluorescein
     126854-14-6 131071-60-8, 3,10-Dihydroxyspiro[7H-benzo[c]xanthene-
                                     131071-61-9, 3,10-Dihydroxyspiro[7H-
     7,1'(3'H)-isobenzofuran]-3'-one
    benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one diacetate
131071-62-0
    131071-68-6, 5'-Carboxy-10-dimethylamino-3-hydroxy-spiro[7H-
    benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one
                                                       131071-69-7,
     3-Acetoxy-5'-acetoxymethoxycarbonyl-10-dimethylaminospiro[7H-
    benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one
                                                        131071-70-0,
     5'-Carboxy-3,10-dihydroxy-spiro[7H-benzo[c]xanthene-7,1'(3'H)-
     isobenzofuran]-3'-one
                             131071-71-1,
6'-Carboxy-9-chloro-3,10-dihydroxy-
     spiro[7H-benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one
131071-76-6,
     6'-Carboxy-10-ethylamino-3-hydroxy-9-methyl-spiro[7H-benzo[c]xanthene-
     7,1'(3'H)-isobenzofuran]-3'-one 131071-80-2,
5'-Carboxy-10-ethylamino-3-
```

hydroxy-9-methyl-spiro[7H-benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one

```
131084-60-1,
6'-Carboxy-3,10-dihydroxy-spiro[7H-benzo[c]xanthene-7,1'(3'H)-
     isobenzofuran]-3'-one 131084-61-2 136832-63-8, 5-
     Chloromethylfluorescein diacetate 142975-81-3, 5-Carboxy-2',7'-
                          144316-86-9, 6-Carboxy-2',7'-dichlorofluorescein
     dichlorofluorescein
     144489-09-8, 5-Carboxy-2',7'-dichlorofluorescein diacetate
144489-10-1,
     6-Carboxy-2',7'-dichlorofluorescein diacetate
                                                     145103-60-2.
     5-Carboxynaphthofluorescein 145103-61-3, 6-Carboxynaphthofluorescein
     145694-94-6,
4-[2-Chloro-6-(ethylamino)-7-methyl-3-oxo-3H-xanthen-9-yl]-
     1,3-benzenedicarboxylic acid 156178-72-2, 5'-Carboxy-3,10-diacetoxy-
     spiro[7H-benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one
164256-07-9,
     5-Carboxynaphthofluorescein diacetate 164256-08-0
                                                          164256-09-1
     164256-10-4
                  164256-11-5
                                 164256-12-6,
6'-Carboxy-3,10-diacetoxyspiro[7H-
     benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one
                                                       164256-13-7,
5'-Carboxy-9-chloro-3,10-dihydroxy-spiro[7H-benzo[c]xanthene-7,1'(3'H)-
     isobenzofuran]-3'-one
                             164256-14-8,
5'-Carboxy-9-chloro-3,10-diacetoxy-
     spiro[7H-benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one
164256-15-9,
6'-Carboxy-9-chloro-3,10-diacetoxy-spiro[7H-benzo[c]xanthene-7,1'(3'H)-
     isobenzofuranl-3'-one
                             164256-16-0,
6'-Carboxy-10-dimethylamino-3-hydroxy-
     spiro[7H-benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-3'-one
164256-17-1,
5'-Carboxy-10-diethylamino-3-hydroxyspiro[7H-benzo[c]xanthene-7,1'(3'H)-
     isobenzofuran]-3'-one 164256-18-2 164256-19-3
                                                        164256-20-6
                  164715-06-4
     164715-05-3
                                 164715-14-4
                                              164715-15-5
     164715-20-2
                                 164906-47-2, 2',7'-Bis-(2-carboxyethyl)-6-
                   164906-46-1
     carboxyfluorescein acetoxymethyl ester
     RL: ARU (Analytical role, unclassified); DEV (Device component use);
ANST
     (Analytical study); USES (Uses)
        (pH sensitive indicator component of sensor with improved drift
        stability)
    ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
L80
              Document No. 119:19371 Air-gap fiber-optic ammonia gas
     sensor. Kar, Satyajit; Arnold, Mark A. (Dep. Chem., Univ. Iowa, Iowa
     City, IA, 52242, USA). Talanta, 40(5), 757-60 (English) 1993. CODEN:
     TLNTA2.
             ISSN: 0039-9140.
AB
     A novel fiber-optics gas sensing arrangement based on an air-gap
```

<WALKE 10/789566><Page 56>

designs is evaluated. In this arrangement, a small gap of air separates

the internal solution from the sample. In addition, a second air-gap separates

the internal solution from a fiber-optic probe measures the fluoroscence of the internal solution. A series of gas sensors for ammonia is

used to investigate several critical design parameters. The length of the

air-gap between the internal solution and the fiber-optic probe affects the magnitude of response. The length of the air-gap separating the

internal and sample solns. has minimal effect on either magnitude or rate

of response. As with membrane-type gas sensors, thickness of the internal

solution and concentration of the indicator **dye** are the most important sensor parameters to consider when designing a fiber-**optic** gas sensor.

IT 100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein 100111-03-3, 6-Carboxy-4',5'-dimethylfluorescein

RL: ANST (Analytical study)

(internal solution containing, in air-gap fiber-optic ammonia gas sensor for anal.)

RN 100111-02-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

RN 100111-03-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

CC 79-2 (Inorganic Analytical Chemistry)

ST air gap fiber optic ammonia sensor

IT Sensors

(gas, fiber-optic, air-gap, for ammonia determination)

IT 7664-41-7, Ammonia, analysis

RL: ANT (Analyte); ANST (Analytical study)

(determination of, air-gap fiber-optic gas sensor for)

IT 3301-79-9, 6-Carboxyfluorescein 12125-02-9, Ammonium chloride, analysis

76823-03-5, 5-Carboxyfluorescein 100111-02-2,

5-Carboxy-4',5'-dimethylfluorescein 100111-03-3,

6-Carboxy-4',5'-dimethylfluorescein

RL: ANST (Analytical study)

(internal solution containing, in air-gap fiber-optic ammonia gas sensor for anal.)

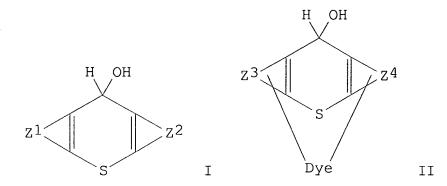
L80 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN 1993:222928 Document No. 118:222928 Photosensitive composition containing

thioxanthen-9-ol derivative and its use for formation of ultraviolet light-cured image for printing plate. Ii, Atsuhiko; Minami, Takahide; Nakamura, Koichi (Kao Corp., Japan). Jpn. Kokai Tokkyo Koho JP 04107559

A2 19920409 Heisei, 13 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP

1990-228800 19900829.

GΙ



AB A photosensitive composition contains a thioxanthenol derivative [I; Z1, Z2 =

(un)substituted benzene or naphthalene ring], a photosensitive resin having a photodimerizable group, and a photoradical generator sensitive to

the visible light region. Alternatively a photosensitive composition contains

a thioxanthenol derivative [II; Dye = a dye bonded to the Z3 and/or Z4 ring,

reacting with a photoradical generator and generating a radical upon irradiation with a light of its absorption wavelength; Z3, Z4 = benzene or

naphthalene ring (un) substituted with a group other than Dye], a photosensitive resin having a photodimerizable group, and a photoradical

generator. A cured image is formed by imagewise irradiation of a visible

light to a photosensitive layer consisting of the above photosensitive composition to form a latent image and irradiation of the entire surface with a UV

light followed by development. The composition gives very sharp images.

IT 145334-72-1 145334-73-2

RL: USES (Uses)

(photosensitive composition containing, for manufacture of printing plate)

RN 145334-72-1 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3',6'-dihydroxy-6-[2-[(9-

hydroxy-9H-thioxanthen-2-yl)oxy]ethoxy]-2',7'-diiodo-4',5'-dimethyl-, disodium salt (9CI) (CA INDEX NAME)

<WALKE 10/789566><Page 59>

●2 Na

RN 145334-73-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 6,6''-[(9-hydroxy-9H-

thioxanthene-2,7-diyl)bis(oxy-2,1-ethanediyloxy)]bis[3',6'-dihydroxy-2',7'-diiodo-4',5'-dimethyl-, tetrasodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

●4 Na

PAGE 1-B

IC ICM G03F007-031

ICS G03F007-027; G03F007-029

CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT Photoimaging compositions and processes

(containing thioxanthenol derivative, for visible light exposure and $\ensuremath{\mathsf{UV}}$

light-cured imaging)

90-93-7, 4,4'-Bisdiethylaminobenzophenone ΙT 90-94-8, Michler's ketone 100-10-7, p-Dimethylaminobenzaldehyde 102-82-9, Tributylamine 103-01-5, N-Phenylglycine 121-69-7, N, N-Dimethylaniline, uses 619-84-1, p-Dimethylaminobenzoic acid 620-40-6, Tribenzylamine 5465-90-7 6783-74-0, Thioxanthen-9-ol 7432-75-9, 12H-Benzo[b]thioxanthen-12-ol 10287-53-3, Ethyl p-dimethylaminobenzoate 14779-78-3, Amyl p-dimethylaminobenzoate 19789-59-4 67362-76-9 143057-50-5 135929-39-4 143057-51-6 143436-29-7 143436-31-1 144092-75-1 144092-73-9, 9H-Thioxanthene-1,9-diol 144092-77-3 144092-78-4 144092-83-1 144092-86-4 144092-82-0 144092-84-2 144092-92-2 144092-95-5 144092-96-6 144092-98-8 144203-59-8 144203-69-0 144203-71-4 145334-67-4 144203-67-8 144203-77-0 145334-69-6 145334-70-9 145334-71-0 **145334-72-1** 145334-73-2 145361-14-4

RL: USES (Uses)

(photosensitive composition containing, for manufacture of printing plate)

L80 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

1992:608461 Document No. 117:208461 optical probe and method for monitoring analyte concentration. Sharma, Ashutosh (Iowa State University Research Foundation, Inc., USA). PCT Int. Appl. WO 9212424 A1

19920723, 40 pp. DESIGNATED STATES: W: AU, CA, JP; RW: AT, BE, CH, DE,

<WALKE 10/789566><Page 61>

DK, ES, FR, GB, GR, IT, LU, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1991-US4015 19910607. PRIORITY: US 1991-638043 19910104.

AB An optical probe for measuring the concentration of an analyte (or partial pressure of a gas) in a sample comprises an indicator matrix containing ≥2 different luminescent (fluorescent or phosphorescent) mols., the luminescence of each of which is quenched by the analyte. Each

of the luminescent mols. has ≥ 1 major band in its absorption spectrum that overlaps with ≥ 1 major band in the absorption spectrum of each of the other luminescent mols., and each of the luminescent mols. has ≥ 1 major band in its emission spectrum that overlaps with ≥ 1 major band in the emission spectrum of each of the other luminescent mols., so that all the luminescent mols. may be coexcited at a common wavelength and the emitted luminescence from

all the mols. can be monitored at a common wavelength. The coexcitation

results
in improved photostability of the mols., since the excitation energy is

shared among the mols. The luminescent mols. may be immobilized on a support and/or enclosed in an analyte-permeable membrane. Thus, a fiber-

optic O sensor had at its tip a disk of filter paper impregnated with 2 fluorescent mols., perylene dibutyrate and decacyclene. The probe,

with excitation at 410 nm and measurement at 510 nm, was highly sensitive

to minute changes in O concentration

IT 100111-02-2, 5-Carboxy-4',5'-dimethylfluorescein
100111-03-3, 6-Carboxy-4',5'-dimethylfluorescein
RL: PROC (Process)

(luminescence quenching of, in pH determination)

RN 100111-02-2 HCAPLUS

CN Spiro(isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

RN 100111-03-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

IC ICM G01N033-00

ICS G01N033-44; G01N021-76

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 80

ST luminescent mol optical probe; fluorescent mol fiber optic probe; oxygen sensor perylene decacyclene

IT Optical detectors

(for chemical anal. by luminescence quenching, multiple luminescent substances in)

IT Fluorescence quenching

Luminescence quenching

Phosphorescence quenching

(in chemical anal., optical detector containing multiple

luminescent

substances for)

IT Fluorescent substances

<WALKE 10/789566><Page 63>

```
(in optical detector, for chemical anal. by fluorescence
        quenching)
ΙT
     Luminescent substances
        (in optical detector, for chemical anal. by luminescence
        quenching)
ΙT
     Phosphorescent substances
        (in optical detector, for chemical anal. by phosphorescence
        quenching)
ΙT
     Gas analysis
        (optical detector for, by luminescence quenching, multiple
        luminescent substances in)
IT
        (triphenylmethane, luminescence quenching of, in sulfur dioxide
determination)
     Unsaturated compounds
ΙT
     RL: ANST (Analytical study)
        (conjugated, luminescent, optical detector containing, for chemical
        anal. by luminescence quenching)
ΙT
     Optical detectors
        (fiber-optic, for chemical anal. by luminescence quenching,
        multiple luminescent substances in)
ΙT
     Porphyrins
     RL: ANST (Analytical study)
        (metal complexes, luminescent, optical detector containing
        multiple, for chemical anal. by luminescence quenching)
     Aromatic hydrocarbons, uses
ΙT
     RL: USES (Uses)
        (polycyclic, luminescent, optical detector containing, for chemical
        anal. by luminescence quenching)
     76-54-0, 2',7'-Dichlorofluorescein 2321-07-5, Fluorescein
3301-79-9,
     6-Carboxyfluorescein
                           76823-03-5 100111-02-2,
     5-Carboxy-4',5'-dimethylfluorescein 100111-03-3,
     6-Carboxy-4',5'-dimethylfluorescein
                                           121535-95-3, 1-
     Hydroxypyrenetrisulfonic acid
                                     142975-81-3, 5-Carboxy-2',7'-
                           144316-86-9, 6-Carboxy-2',7'-dichlorofluorescein
     dichlorofluorescein
     RL: PROC (Process)
        (luminescence quenching of, in pH determination)
    ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN
1992:556559
              Document No. 117:156559 Indicators for the optical
     measurement of sulfur dioxide gas. Sharma, Ashutosh; Ali, Zulfigur;
     McStay, Daniel (Opt. Diagn. Biotechnol. Cent., Cranfield Inst.
Technol.,
     Cranfield/Bedfordshire, MK43 OAL, UK). Proceedings of SPIE-The
    International Society for Optical Engineering, 1637 (Enrion. Process
Monit.
     Technol.), 280-4 (English) 1992. CODEN: PSISDG. ISSN: 0277-786X.
```

<WALKE 10/789566><Page 64>

AB A number of fluorophores were examined for their suitability as indicators in

SO2 measurement. Several indicators, including polycyclic aromatic hydrocarbons, 5- and 6-carboxy-4',5'-dimethyl fluorescein, new fuchsin,

hydrazine hydrochloride, and chloropyridine hydrochloride, decreased the

fluorescence intensity with an increase in SO2 concentration Fluorescence

quenching of benzopurpurine is extremely efficient, with little or no interference from NH3 and H2S. Stern-Volmer plots of quenching were used

to determine quenching consts. A fiber optic SO2 sensor/probe based on these findings is under development.

IT 100111-02-2 100111-03-3

RL: ANST (Analytical study)

(fluorophore, for sulfur dioxide determination in air)

RN 100111-02-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

RN 100111-03-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

CC 59-1 (Air Pollution and Industrial Hygiene)

Section cross-reference(s): 79

IT Sensors

(gas, fiber-optic, for sulfur dioxide determination, by fluorescence

quenching)

IT 992-59-6, Benzopurpurine 4B 3248-91-7 7379-35-3 14011-37-1,

Hydrazine hydrochloride 100111-02-2 100111-03-3

Ι

RL: ANST (Analytical study)

(fluorophore, for sulfur dioxide determination in air)

L80 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN 1988:429996 Document No. 109:29996 Silver halide color photographic material

containing leuco dyes, reducing agent, and polymerizable material. Harada, Toru; Sato, Kozo (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai

Tokkyo Koho JP 62288828 A2 19871215 Showa, 24 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1986-133092 19860609.

GΙ

$$\begin{array}{c|c} R^{10} & O & OR^{2} \\ \hline R^{3}_{b} & A & R^{4}_{c} \\ \hline \end{array}$$

ΙI

<WALKE 10/789566><Page 66>

AB A color photog. material having a high signal/noise ratio is claimed which

comprises a support, Ag halide, a reducing agent, a polymerizable material, and a leuco dye I or II [A = 0, NClH4Ra; R = group having a σ (substituent > 0; R1, R2 = (cyclo)alkyl, aralkyl; R3,R4 = (cyclo)alkyl, aralkyl, alkoxy, aryoxy; a, b, c = 1, 2].

IT 115128-15-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and reaction of, leuco dye from, color photog.

material containing

reducing agent, polymerizable material and)

RN 115128-15-9 HCAPLUS

CN Spiro[furo[3,4-b]pyridine-7(5H),9'-[9H]xanthen]-5-one, 2',7'-dihexyl-3',6'-dihydroxy- (9CI) (CA INDEX NAME)

Me-
$$(CH_2)$$
 5 N O (CH_2) 5-Me

IC ICM G03C001-68

ICS G03C001-00; G03C001-02

CC 74-2 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 115128-15-9P 115128-16-0P 115147-61-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and reaction of, leuco dye from, color photog.

material containing

reducing agent, polymerizable material and)

=> => d his 184-

<WALKE 10/789566><Page 67>

FILE 'REGISTRY' ENTERED AT 14:55:02 ON 10 DEC 2004 L84 1 S 87569-95-7 1 S 2321-07-5 L85 L86 1 S 17372-87-1 FILE 'HCAPLUS' ENTERED AT 14:55:42 ON 10 DEC 2004 8267 S L84 OR L85 OR L86 L87 8266 S L85 OR L86 L88 L89 28 S L82 NOT L88 => d 189 1-28 cbib abs hitstr hitind ANSWER 1 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 2004:17479 Document No. 140:70977 Method of measuring drug-metabolizing enzyme activity, method of evaluating inhibition of drug-metabolizing enzyme activity, and composition for these methods. Matsui, Kazuhiro; Ishibashi, Takuya; Oka, Masanori (Toyo Boseki Kabushiki Kaisha, Japan). Eur. Pat. Appl. EP 1378751 A2 20040107, 39 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK. (English). CODEN: EPXXDW. APPLICATION: EP 2003-14486 20030702. PRIORITY: JP 2002-193795 20020702; JP 2002-193796 20020702; JP 2002-229065 20020806; JP 2002-229066 20020806; JP 2002-229067 20020806. The present invention provides a method of measuring drug-metabolizing AB enzyme activity, wherein a drug-metabolizing enzyme is first applied to a substrate (particularly an endogenous unmodified substrate), and measurement is performed preferably within three hours by immunochem. assay of the resulting product. ΙT 70672-05-8 RL: BSU (Biological study, unclassified); BIOL (Biological study) (substrate; method of measuring drug-metabolizing enzyme activity and method of evaluating inhibition of drug-metabolizing enzyme activity and composition for these methods) 70672-05-8 HCAPLUS RN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, CN 3'-hydroxy-6'-methoxy-(9CI) (CA INDEX NAME)

IC ICM G01N033-53

ICS G01N033-543

CC 1-2 (Pharmacology)

Section cross-reference(s): 2, 7

IT 50-12-4, Mephenytoin 52-86-8, Haloperidol 53-16-7, Estrone, biological

studies 53-35-0, 6β -Hydroxycortisol 57-83-0, Progesterone, biological studies 58-08-2, Caffeine, biological studies 58-22-0, Testosterone 63-05-8, Androstenedione 64-77-7, Tolbutamide 80-08-0,

Dapsone 103-90-2, Acetaminophen 521-18-6, Dihydrotestosterone 581-88-4, Debrisoquine sulfate 3066-12-4, 11α -Hydroxytestosterone 5543-57-7, (S)-Warfarin 5543-58-8, (R)-Warfarin 5725-89-3, Methoxyresorufin 15307-86-5, Diclofenac 18609-21-7,

Dextromethorphan

and

hydrochloride 27203-92-5, Tramadol 33069-62-4, Taxol 54340-62-4, Bufuralol 59467-70-8, Midazolam 65846-44-8 70672-05-8 73590-58-6, Omeprazole 115453-82-2,

7-Ethoxy-4-trifluoromethylcoumarin

117620-77-6 131802-60-3, 7-Benzyloxyquinoline 641629-24-5 641629-25-6

RL: BSU (Biological study, unclassified); BIOL (Biological study) (substrate; method of measuring drug-metabolizing enzyme activity

method of evaluating inhibition of drug-metabolizing enzyme activity

and composition for these methods)

L89 ANSWER 2 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 2003:904195 Document No. 140:245948 Identification of gap junction blockers

using automated fluorescence microscopy imaging. Li, Zhuyin; Yan, Yongping; Powers, Elaine A.; Ying, Xiaoyou; Janjua, Khurram; Garyantes, Tina; Baron, Bruce (Lead Discovery Technology, Lead tration.

Aventis Pharmaceutical, Bridgewater, NJ, USA). Journal of Biomolecular

Screening, 8(5), 489-499 (English) 2003. CODEN: JBISF3. ISSN: 1087-0571.

Publisher: Sage Publications.

AB Gap junctions coordinate elec. signals and facilitate metabolic synchronization between cells. In this study, the authors have developed

a novel assay for the identification of gap junction blockers using fluorescence microscopy **imaging**-based high-content screening technol. In the assay, the communication between neighboring cells through gap junctions was measured by following the redistribution of

a

fluorescent marker. The movement of calcein dye from dye-loaded donor cells to dye-free acceptor cells through gap junctions overexpressed on cell surface membranes was monitored using automated fluorescence microscopy imaging in a high-throughput compatible format. The fluorescence imaging technol. consisted of automated focusing, image acquisition, image processing, and data mining. The authors have successfully performed

а

high-throughput screening of a 486,000- compound program with this assay,

and they were able to identify false positives without addnl. expts. Selective and pharmacol. interesting compds. were identified for further

optimization.

IT 1461-15-0, Calcein

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(identification of gap junction blockers using automated fluorescence

microscopy imaging)

RN 1461-15-0 HCAPLUS

CN Glycine, N,N'-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2',7'-diyl)bis(methylene)]bis[N-(carboxymethyl)-(9CI)(CA

INDEX NAME)

$$HO_2C-CH_2$$
 CH_2-CO_2H $CH_2-N-CH_2-CO_2H$

CC 1-1 (Pharmacology) ΙΤ Imaging (fluorescent; identification of gap junction blockers using automated fluorescence microscopy imaging) ΙT Cell junction (gap junction; identification of gap junction blockers using automated fluorescence microscopy imaging) ΤT Fluorescent substances High throughput screening Optical imaging devices (identification of gap junction blockers using automated fluorescence microscopy imaging) ΙT 1461-15-0, Calcein RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (identification of gap junction blockers using automated fluorescence microscopy imaging) ANSWER 3 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 2002:693235 Document No. 137:213266 Non-separation assay method and system using opaque particles. Cassells, John; Cope, Tristan John (The Technology Partnership Public Limited Company, UK). Eur. Pat. Appl. EΡ 1239284 A1 20020911, 17 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR. (English). CODEN: EPXXDW. APPLICATION: EP 2001-302110 20010308. A method for performing a non-separation assay for determining the AB level of binding of one component to another. A first component is provided incorporating a fluorescent probe dissolved or suspended in solution A substantially opaque particle is provided onto or into which is incorporated binding sites for the first component and optionally incorporating a dye or fluorophore of different emission spectrum to the first component. The opaque particle is immersed in a solution or suspension of the first component, and the opaque particle to settle out of the solution, or

be

<WALKE 10/789566><Page 71>

transported to a fixed position by an applied force. The solution and opaque

particle are illustrated with a beam of light such that the opaque particle is in the foreground and attenuates and illuminating beam before

it passes into the solution beyond. The intensity of received light (fluorescence) from the first component over an area of the sample with an

imaging or scanning detector from the same side of the sample as
 the illuminating light is determined, and the position of the second
component

in the sample is determined by detecting attenuation of the received light from $% \left(1\right) =\left(1\right) +\left(1\right) +\left($

the sample and/or by detecting the presence of received light from a dye incorporated in the second component. An apparatus, as well as opaque particles for performing the method are also provided.

IT 27072-45-3, Fluorescein isothiocyanate

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (non-separation assay method and system using opaque particles)

RN 27072-45-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-5(or 6)-isothiocyanato- (9CI) (CA INDEX NAME)

D1-N=C=S

IC ICM G01N033-53

ICS G01N033-543; G01N033-58; G01N033-542

CC 9-16 (Biochemical Methods)

IT Analytical apparatus

Cell membrane

Centrifugation

Density

Dissolution

Dyes

```
Electric charge
     Electrophoresis
     Electrostatic charge
     Emission spectra
    Eubacteria
     Fluorescence
     Fluorescent indicators
     Fluorescent substances
     Force
     Gravity
     Illumination
       Imaging
     Light
    Magnetic field
    Magnetic particles
    Molecules
       Optical imaging devices
     Samples
     Sensors
     Separation
     Solutions
     Suspensions
     Virus
     Volume
     Wavelength
    Wetting
        (non-separation assay method and system using opaque particles)
     27072-45-3, Fluorescein isothiocyanate
     RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
        (non-separation assay method and system using opaque particles)
    ANSWER 4 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN
2002:578876
            Document No. 138:267841 Fluorescence data analysis on
gel-based
     biochips. Barsky, Victor; Perov, Alexander; Tokalov, Sergei;
Chudinov,
     Alexander; Kreindlin, Edward; Sharonov, Alexei; Kotova, Ekaterina;
    Mirzabekov, Andrei (Engelhardt Institute of Molecular Biology, Russian
     Academy of Sciences, Moscow, Russia). Journal of Biomolecular
Screening,
     7(3), 247-257 (English) 2002. CODEN: JBISF3. ISSN: 1087-0571.
     Publisher: Mary Ann Liebert, Inc..
     A series of biochip readers developed for gel-based biochips includes
     three imaging models and a novel nonimaging biochip scanner.
     The imaging readers, ranging from a research-grade versatile
     reader to a simple portable one, use wide-field objectives and 12-bit
```

digital large-coupled device cameras for parallel addressing of

ΙT

AB

multiple

<WALKE 10/789566><Page 73>

array elements. This feature is valuable for monitoring the kinetics of

sample interaction with immobilized probes. Depending on the model and

the label used, the sensitivity of these readers approaches 0.3 amol of a $\,$

labeled sample per gel element. In the selective scanner, both the spot

size of the excitation laser beam and the detector field of view match the $\,$

size of the biochip array elements so that the whole row of the array can

be read in a single scan. The portable version reads 50-mm long, 150-element, one-dimensional arrays in 5 s. With a dynamic range of 4000:1, a sensitivity of 1-5 amol of a labeled sample per gel element, and

a data format facilitating online processing, the scanner is an attractive, inexpensive solution for biomedical diagnostics.

for sample labeling were compared exptl. in terms of detection sensitivity, influence on duplex stability, and suitability for multilabel

anal. and thermodn. studies. Texas Red and tetracarboxyphenylporphyn proved to be the best choice for two-wavelength anal. using the imaging readers.

IT 27072-45-3, Fluorescein isothiocyanate

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (imaging and nonimaging fluorescent biochip readers for gel-based biochips and comparison of fluorescent dyes)

RN 27072-45-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-5(or 6)-isothiocyanato- (9CI) (CA INDEX NAME)

$$D1 - N = C = S$$

```
9-1 (Biochemical Methods)
CC
ΙT
     Imaging
       Optical imaging devices
        (fluorescent; imaging and nonimaging fluorescent biochip
        readers for gel-based biochips and comparison of fluorescent
        dyes)
ΙT
     CCD cameras
     Fluorescent dyes
     Microarray technology
     Optical scanners
        (imaging and nonimaging fluorescent biochip readers for
        gel-based biochips and comparison of fluorescent dyes)
ΙT
     DNA
     Oligonucleotides
     RL: ANT (Analyte); ANST (Analytical study)
        (imaging and nonimaging fluorescent biochip readers for
        gel-based biochips and comparison of fluorescent dyes)
ΙT
     14609-54-2 27072-45-3, Fluorescein isothiocyanate
                                                         70281-37-7,
     Tetramethylrhodamine
                           82354-19-6, Texas Red
                                                    113078-49-2
146368-14-1
                                            209340-49-8, BODIPY 630/650
     146368-16-3
                   165599-63-3, BODIPY FL
     RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
        (imaging and nonimaging fluorescent biochip readers for
        gel-based biochips and comparison of fluorescent dyes)
    ANSWER 5 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN
2002:256575
              Document No. 136:275685 Quantitative digital fluorography
and
     related products and methods. Botz, Eduard J.; Rana, Victoriano F.;
    Newton, Kenneth R.; Lin, Tsue-ming (Hyperion, Inc., USA). PCT Int.
Appl.
     WO 2002027296 A1 20020404, 26 pp. DESIGNATED STATES: W: AE, AG, AL,
AM,
    AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE,
DK,
     DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
KE,
     KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,
MX,
    MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
TZ,
     UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM;
RW:
     AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB,
GR,
     IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English).
     CODEN: PIXXD2. APPLICATION: WO 2001-US42219 20010917. PRIORITY: US
```

2000-671956 20000927.

AB The present invention thus relates to marker components, fluorescent probes, oligonucleotides, hybridization assays, and binding assays such as

immunoassays, DNA assays and receptor assays using such products and methods for making such products. According to the present invention, delectably labeled marker components are provided thus comprise a fluorophore moiety coupled to two or more small solubilizing axial ligands, which preferably reduce or remove the problems of solvent sensibility and non-specific binding.

IT **27072-45-3**, Fitc

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (quant. digital fluorog. and related products and methods)

RN 27072-45-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-5(or 6)-isothiocyanato- (9CI) (CA INDEX NAME)

$$D1 - N = C = S$$

IC ICM G01N015-14

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 3, 14, 15

IT Electrooptical imaging devices

(digital cameras; quant. digital fluorog. and related products and methods)

IT Imaging

(luminescence; quant. digital fluorog. and related products and methods)

IT AIDS (disease)

Algorithm

Animal tissue

Autoimmune disease

Body fluid

CCD cameras

Calibration Cell nucleus Chlamydia Classification Coupling reaction Crosslinking Cytomegalovirus Cytoplasm DNA microarray technology Diagnosis Dot blot hybridization Drying Fluorescence Fluorescent dyes Fluorescent indicators Fluorescent substances Granulomatous disease Herpesviridae Human

Imaging

Immobilization, molecular or cellular Immunoassay Infection
Least squares method
Liquids
Luminescence
Luminescent substances
Lyme disease
Mathematical methods
Microarray technology
Microtiter plates
Neutrophil
Northern blot hybridization
Nucleic acid hybridization
Optical absorption

Optical imaging devices

Pathogen
Photodiodes
Photomultipliers
Prokaryota
Rheumatoid arthritis
Robotics
Rubella
Samples
Solids
Solubilization
Solvents
Southern blot hybridization

<WALKE 10/789566><Page 77>

Suspensions Video cameras Virus Washing Wavelength

(quant. digital fluorog. and related products and methods) IT 27072-45-3, Fitc

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (quant. digital fluorog. and related products and methods)

L89 ANSWER 6 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 2001:453279 Document No. 135:57846 Diethoxyfluorescein as a substrate for

human cytochrome P 450 and use of diethoxyfluorescein for high throughput

inhibition screening assays. Bambal, Ramesh; Bloomer, Jacqueline Carol

(Smithkline Beecham P.L.C., UK; Smithkline Beecham Corporation). PCT Int.

Appl. WO 2001044495 A2 20010621, 9 pp. DESIGNATED STATES: W: AE, AG, AL,

AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE,

DK,

DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,

KE,

KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,

MX,

UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM;

MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,

RW:

AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB,

GR,

IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-EP12450 20001208. PRIORITY: US 1999-PV170405 19991213.

AB Diethoxyfluorescein has been identified as a general substrate for human

cytochrome P 450. In particular diethoxyfluorescein is an improved substrate for human cytochrome P 450 3A4 (CYP3A4) and cytochrome P 450 2C8

(CYP2C8), which is of use for configuring high throughput inhibition screening assays. An assay for identifying inhibitors of human cytochrome

P 450 using diethoxyfluorescein as the substrate and measuring inhibition

of O-dealkylation of diethoxyfluorescein by the enzyme. The readily quantifiable fluorescent product can be scanned.

IT 87569-95-7

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);

MFM (Metabolic formation); THU (Therapeutic use); ANST (Analytical study);

BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses) (diethoxyfluorescein as substrate for human cytochrome P 450 and use of

diethoxyfluorescein for high throughput inhibition screening assays)

RN 87569-95-7 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3'-ethoxy-6'-hydroxy-(9CI) (CA INDEX NAME)

IC ICM C120001-00

CC 7-1 (Enzymes)

Section cross-reference(s): 1

IT 87569-95-7

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);

MFM (Metabolic formation); THU (Therapeutic use); ANST (Analytical study);

BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses) (diethoxyfluorescein as substrate for human cytochrome P 450 and use of

diethoxyfluorescein for high throughput inhibition screening assays)

L89 ANSWER 7 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

2001:453254 Document No. 135:56900 Production with recombinant cells of human cdc25 phosphatases fused with MBP and method for identifying human

cdc25 phosphatase modulators. Goubin-Gramatica, Francoise; Ducommun, Bernard; Prevost, Gregoire (Societe de Conseils de Recherches et d'Applications Scientifiques (S.C.R.A.S.), Fr.). PCT Int. Appl. WO 2001044467 A2 20010621, 55 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT,

<WALKE 10/789566><Page 79>

```
AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM,
DZ,
     EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,
KP,
     KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ,
NO,
     NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
UG,
     US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT,
BE,
     BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE,
IT,
     LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR.
                                                       (French).
                                                                  CODEN:
PIXXD2.
     APPLICATION: WO 2000-FR3496 20001213. PRIORITY: FR 1999-15722
19991214;
     FR 2000-6883 20000530; FR 2000-12008 20000921.
```

AB The invention concerns a method for obtaining human Cdc25B1, Cdc25B2, Cdc25B3 and Cdc25C phosphatases. More particularly, the invention concerns a fusion between human Cdc25B1, Cdc25B2, Cdc25B3 or Cdc25C phosphatase and the maltose binding protein (MBP) of Escherichia coli, the

DNAs coding for said fusion proteins, a method for preparing said fusion

proteins, and a method for identifying human Cdc25B1, Cdc25B2, Cdc25B3 or

 $\tt Cdc25C$ protein modulators. Thus, a plasmid containing a gene for E. coli MBP

fused to human CDC25C was constructed. E. coli transformed with this plasmid was cultured to produce the fusion protein, which was isolated using an amylose-agarose affinity column.

IT 70672-05-8

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (production with recombinant cells of human cdc25 phosphatases fused with

MBP and method for identifying human cdc25 phosphatase modulators) RN 70672-05-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3'-hydroxy-6'-methoxy-

(9CI) (CA INDEX NAME)

IC ICM C12N015-12

GΙ

ICS C12N009-16; C07K014-47; C12N015-62; C12Q001-42

CC 3-2 (Biochemical Genetics)

Section cross-reference(s): 7

IT 21214-18-6 70672-05-8

OH

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (production with recombinant cells of human cdc25 phosphatases fused with

MBP and method for identifying human cdc25 phosphatase modulators)

L89 ANSWER 8 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 1999:306617 Document No. 131:127297 Synthesis of a new fluorogenic substrate

for the continuous assay of mammalian phosphoinositide-specific phospholipase C. Rukavishnikov, Aleksey V.; Zaikova, Tatiana O.; Birrell,

G. Bruce; Keana, John F. W.; Griffith, O. Hayes (Department of Chemistry,

University of Oregon, Eugene, OR, 97403, USA). Bioorganic & Medicinal Chemistry Letters, 9(8), 1133-1136 (English) 1999. CODEN: BMCLE8. ISSN:

0960-894X. Publisher: Elsevier Science Ltd..

Ι

AB The synthesis of a fluorogenic substrate (I) for mammalian phosphoinositide-specific phospholipase C is described. I, based on the

widely used fluorescein mol., is a water-soluble substrate analog of phosphatidylinositol-4-phosphate. I is shown to be a sensitive substrate

for human PI-PLC- δ 1 in a continuous assay.

IT 214745-51-4

of

of

RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of a new fluorogenic substrate for the continuous assay

mammalian phosphoinositide-specific phospholipase C)

RN 214745-51-4 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3'-(hexyloxy)-6'-hydroxy-(9CI) (CA INDEX NAME)

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 7, 33

IT 119874-35-0 **214745-51-4**

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis of a new fluorogenic substrate for the continuous assay

mammalian phosphoinositide-specific phospholipase C)

L89 ANSWER 9 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1998:731807 Document No. 129:348963 Spectrally tuned multiple bandpass filters for video displays. Teng, Chia-Chi; Suh, Suk Youn; Yoon, Hyun-Nam

(Hoechst Celanese Corp., USA). U.S. US 5834122 A 19981110, 7 pp. (English). CODEN: USXXAM. APPLICATION: US 1996-753349 19961125.

AB Multiple band pass filters for contrast enhancement of color displays are

described which comprise a uniform layer having a plurality of selectively

<WALKE 10/789566><Page 82>

transmitting and absorbing dyes intermixed in a polymer matrix. IT 3326-34-9 18472-87-2, Phloxine B

RL: DEV (Device component use); USES (Uses) (spectrally tuned multiple bandpass filters based on dye -containing polymer compns. for video displays)

RN 3326-34-9 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

5-amino-3',6'-dihydroxy-

(9CI) (CA INDEX NAME)

RN 18472-87-2 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,
2',4',5',7'-tetrabromo-

4,5,6,7-tetrachloro-3',6'-dihydroxy-, disodium salt (9CI) (CA INDEX NAME)

```
TC
     ICM G02B001-10
     ICS G02B001-11; G02B005-20
NCL
     428412000
CC
     73-11 (Optical, Electron, and Mass Spectroscopy and Other Related
     Properties)
     Section cross-reference(s): 74
     Polyesters, uses
ΙT
     Polyesters, uses
     RL: DEV (Device component use); USES (Uses)
        (polyamide-; spectrally tuned multiple bandpass filters based on
        dye-containing polymer compns. for video displays)
ΙT
     Polyamides, uses
     Polyamides, uses
     RL: DEV (Device component use); USES (Uses)
        (polyester-; spectrally tuned multiple bandpass filters based on
        dye-containing polymer compns. for video displays)
     Cycloalkenes
ΙT
     RL: DEV (Device component use); USES (Uses)
        (polymers; spectrally tuned multiple bandpass filters based on
        dye-containing polymer compns. for video displays)
IT
     Optical imaging devices
        (spectrally tuned multiple bandpass filters based on dye
        -containing polymer compns. for)
ΙT
     Optical filters
        (spectrally tuned multiple bandpass filters based on dye
        -containing polymer compns. for video displays)
ΙT
     Acrylic polymers, uses
     Polyamides, uses
     Polycarbonates, uses
     Polyesters, uses
     Polyethers, uses
     Polyketones
     Polyolefins
     Polyurethanes, uses
     RL: DEV (Device component use); USES (Uses)
        (spectrally tuned multiple bandpass filters based on dye
       -containing polymer compns. for video displays)
                                                 9002-89-5, Polyvinyl
ΙT
     1330-38-7, Luxol Fast Blue MBSN 3326-34-9
               9003-20-7, Polyvinyl acetate
                                              9003-53-6, Polystyrene
     18472-87-2, Phloxine B
                             60311-02-6, Sulforhodamine 101
     RL: DEV (Device component use); USES (Uses)
        (spectrally tuned multiple bandpass filters based on dye
        -containing polymer compns. for video displays)
    ANSWER 10 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN
1998:608674
              Document No. 129:213838 Optical membrane films for
polycation
```

detection and application to protamine determination. Wang, Enju (St.

<WALKE 10/789566><Page 84>

John's University, USA). PCT Int. Appl. WO 9838263 Al 19980903, 40 pp.

DESIGNATED STATES: W: CA, JP; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,

IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO

1998-US4004 19980227. PRIORITY: US 1997-39464 19970227.

AB Lipophilic fluorescein-based mols. have been synthesized and incorporated

into thin plasticized polymeric membrane films as chromoionophores for the ${}^{\circ}$

optical sensing and detection of polycationic protamine. The membrane response is based on the extraction of protamine into the film due to the

interaction between the anionic fluorescein and the protamine polycation

which results in a cation exchange between the protamine and proton, and

thus, induces an absorbance spectra change of the polymeric film. The response speed is controlled by protamine diffusion through the stagnant

diffusion layer adjacent to the film surface as well as within the bulk of

the polymer film. When limited exposure time and non-stirring detection

modes are used in a buffer solution, absorbance of a film changes as a function of the protamine concentration in the range of about 2 to 60- $\mu g/mL$

(0.44 to 13.3 $\mu M)$. The sensing film shows good selectivity over most common small cations, it can be used in the determination of protamine in diluted

serum or whole blood. No response is observed when a protamine complexing

reagent such as heparin is present, thus the instant invention is useful

as an indicator for the protamine-heparin titration

IT 212632-14-9P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(optical membrane films for polycation detection and application to protamine determination)

RN 212632-14-9 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 5(or 6)-amino-3'-(docosyloxy)-6'-hydroxy-(9CI) (CA INDEX NAME)

$D1-NH_2$

IC ICM C09K003-00

at

ICS F21V009-00; C12Q001-00; C12Q001-37

CC 9-1 (Biochemical Methods)

IT 184423-23-2P, Benzoic acid,

2-(2,7-dichloro-6-hydroxy-3-oxo-3H-xanthen-9-

yl)-, octadecyl ester 212632-11-6P 212632-14-9P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(optical membrane films for polycation detection and application to protamine determination)

L89 ANSWER 11 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 1998:256331 Document No. 128:308397 Preparation of fluorescein monoethers.

Fujita, Satoshi; Yu, Takeshi (Aisin Seiki Co., Ltd., Japan). Jpn. Kokai

Tokkyo Koho JP 10109990 A2 19980428 Heisei, 9 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1996-281714 19961002.

AB Title compds. are prepared by etherification of fluoresceins with n mol

equivalent halo compds. (1 \leq n < 2) in the presence of \geq 1 mol equivalent basic compds. in solvents at 20-35° and treatment with acids. Fluorescein isocyanate was treated with 3,5-xylidine in EtOH

room temperature for 18 h to give 100% N-(3,5-dimethylphenyl)-5-thioureidofluorescein, which was treated with 3,4-dimethylbenzyl chloride

in the presence of K2CO3 in DMF at room temperature for 2 h to give 99.2%

3'-O-N-(3,5-dimethylphenyl) methyl-N-(3,5-dimethylphenyl)-5-thioureidofluorescein.

IT 186187-60-0P 186187-63-3P 190899-06-0P

<WALKE 10/789566><Page 86>

206255-96-1P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of fluorescein monoethers by etherification of fluoresceins

with halo compds.)

RN 186187-60-0 HCAPLUS

[1,1'-Biphenyl]-4-carboxamide, N-[3'-[(3,4-dimethylphenyl)methoxy]-6'-CN hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI)

(CA INDEX NAME)

RN 186187-63-3 HCAPLUS

[1,1'-Biphenyl]-4-carboxamide, CN

N-[3'-hydroxy-6'-(1-naphthalenylmethoxy)-3oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)

RN 190899-06-0 HCAPLUS
CN Thiourea,
N-(3,5-dimethylphenyl)-N'-[3'-[(3,4-dimethylphenyl)methoxy]-6'hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI)
(CA
INDEX NAME)

RN 206255-96-1 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide,
N-[3'-(1-anthracenylmethoxy)-6'-hydroxy-3oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)

IC ICM C07D493-10

ICS C09K011-06

CC 27-14 (Heterocyclic Compounds (One Hetero Atom))

IT 186187-60-0P 186187-63-3P 190899-06-0P

202747-88-4P 202747-89-5P 206255-94-9P 206255-95-0P

206255-96-1P 206255-97-2P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of fluorescein monoethers by etherification of fluoresceins

with halo compds.)

L89 ANSWER 12 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1998:256232 Document No. 129:14204 Assay of nucleic acids, etc., using peroxidase and fluorescent substrates, and peroxidase for it. Fujita, Satoshi; Kagiyama, Naoto; Momiyama, Masayoshi; Kondo, Yasumitsu; Nishiyanai, Miho (Aisin Seiki Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho

JP 10108693 A2 19980428 Heisei, 13 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1996-283143 19961004.

AB Nucleic acids, protein, microorganisms, etc., are assayed by binding peroxidase to them, reacting the peroxidase-labeled analytes with fluorescent substrates, irradiating the reaction products with exciting

light, and detecting the fluorescence. Also claimed is peroxidase used $% \left(1\right) =\left(1\right) +\left(1\right) +\left($

for the assay. Fifteen fluorescence substrates used for the assay are

also disclosed, and some of them are deacetylated by alkaline hydrolysis prior $% \left(1\right) =\left(1\right) +\left(1\right) +\left($

to treating with peroxidase-labeled analytes. The assay method exhibited

good spacial resolution and sensitivity. Detection of λDNA by spotting digoxigenin-labeled λDNA on a nitrocellulose membrane, treating the spotted area with peroxidase-labeled anti-digoxigenin antibodies, dropping an EtOH solution containing Fast Violet B base and H2O2 to

the membrane, and measuring fluorescence was shown.

IT 186187-63-3P

RL: ARG (Analytical reagent use); PNU (Preparation, unclassified); ANST

(Analytical study); PREP (Preparation); USES (Uses)
(assay of nucleic acids and proteins and microorganisms using peroxidase and fluorescent substrates)

RN 186187-63-3 HCAPLUS

CN [1,1'-Biphenyl]-4-carboxamide,

N-[3'-hydroxy-6'-(1-naphthalenylmethoxy)-3oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)

IT 186187-60-0P 190899-06-0P 207671-33-8P 207671-40-7P

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation);

RACT (Reactant or reagent)

(assay of nucleic acids and proteins and microorganisms using

<WALKE 10/789566><Page 90>

peroxidase and fluorescent substrates)

RN 186187-60-0 HCAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[3'-[(3,4-dimethylphenyl)methoxy]-6'-hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI)

(CA INDEX NAME)

RN 190899-06-0 HCAPLUS

CN Thiourea,

N-(3,5-dimethylphenyl)-N'-[3'-[(3,4-dimethylphenyl)methoxy]-6'hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA

INDEX NAME)

Me
$$CH_2-O$$
 OH Me $NH-C-NH$ OH

RN 207671-33-8 HCAPLUS

CN [1,1'-Biphenyl]-4-carboxamide,

N-[3'-(9-anthracenylmethoxy)-6'-hydroxy-3oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX

NAME)

RN 207671-40-7 HCAPLUS
CN Thiourea, N-(3,5-dimethylphenyl)-N'-(3'-ethoxy-6'-hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (9CI) (CA INDEX NAME)

```
IC
     ICM
          C12Q001-28
     ICS
          G01N021-78
CC
     9-5 (Biochemical Methods)
                    186187-55-3P 186187-63-3P
ΙT
     184476-27-5P
                                                188007-69-4P
     207671-30-5P
                    207671-31-6P
                                   207671-32-7P
                                                  207671-34-9P
207671-35-0P
     207671-37-2P
                    207671-38-3P
                                   207671-39-4P
                                                  207671-41-8P
     RL: ARG (Analytical reagent use); PNU (Preparation, unclassified);
ANST
     (Analytical study); PREP (Preparation); USES (Uses)
```

(assay of nucleic acids and proteins and microorganisms using peroxidase and fluorescent substrates)

IT 14002-51-8P, [1,1'-Biphenyl]-4-carbonyl chloride 186187-60-0P 190899-06-0P 202747-88-4P 202747-89-5P 207671-33-8P 207671-40-7P

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP
(Preparation);

RACT (Reactant or reagent)

(assay of nucleic acids and proteins and microorganisms using peroxidase and fluorescent substrates)

L89 ANSWER 13 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 1998:236207 Document No. 129:1978 Measurement of Na+,K+-ATPase activity in

human skeletal muscle. Fraser, Steve F.; McKenna, Michael J. (Department

of Human Movement, Recreation, and Performance, Centre for Rehabilitation,

Exercise, and Sport Science, Victoria University of Technology, Melbourne,

8001, Australia). Analytical Biochemistry, 258(1), 63-67 (English) 1998.

CODEN: ANBCA2. ISSN: 0003-2697. Publisher: Academic Press.

AB There are few published measures of Na+,K+-ATPase activity in human skeletal muscle. This study investigated the suitability of the K+-stimulated 3-O-methylfluorescein phosphatase assay for measurement of

Na+,K+-ATPase activity in human skeletal muscle. Factors investigated include enzyme kinetics, sample treatment, and ligand concentration The addition of

ouabain blocked maximal K+-stimulated 3-0-methylfluorescein phosphatase

(3-O-MFPase) activity, confirming the specificity of the assay. Activity

was \max maximal using a multiple freeze-thaw treatment of the homogenate, a 10

 $\,$ mM KCI activating concentration, and a 3-0-methylfluorescein phosphatase

substrate concentration of 160 μM , which is eight times higher than previously

reported. From quadriceps muscle biopsies taken from seven healthy untrained subjects, the maximal K+-stimulated 3-O-MFPase activity determined

from the homogenates was (mean \pm SE) 292 \pm 10 nmol min-1 \cdot

g-1 wet weight (1745 \pm 84 pmol min-1 \cdot mg-1 protein). This value is five times greater than previously published data for human skeletal

muscle. The intra-assay variability was 8.1% and the interassay

variability was 5.3%. These modifications greatly enhanced the 3-O-MFPase

assay, with the improved enzymic conditions allowing valid, reliable measurement of Na+,K+-ATPase activity in small samples of human skeletal

muscle.

IT 70672-05-8

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (determination of Na+,K+-ATPase activity in human skeletal muscle by a modified

K+-stimulated 3-O-methylfluorescein phosphatase assay)

RN 70672-05-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3'-hydroxy-6'-methoxy-

(9CI) (CA INDEX NAME)

CC 7-1 (Enzymes)

IT 70672-05-8

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (determination of Na+,K+-ATPase activity in human skeletal muscle by a modified

K+-stimulated 3-O-methylfluorescein phosphatase assay)

L89 ANSWER 14 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 1998:151297 Document No. 128:201777 Automatic DNA sequencer and genotyper

having extended spectral response. Dabiri, Ali; Garner, Harold R. (Science Applications International Corporation, USA; Board of Regents,

University of Texas System; Dabiri, Ali; Garner, Harold R.). PCT Int. Appl. WO 9808085 A1 19980226, 41 pp. DESIGNATED STATES: W: AL, AM, AT,

AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB,

GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,

<WALKE 10/789566><Page 94>

MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,

TJ, TM, TR, TT, UA, UG, US, UZ, VN, ZW, AM, AZ, BY, KG, KZ, MD, RU,

TJ,

TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA,

GB,
GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English).
CODEN: PIXXD2. APPLICATION: WO 1997-US14642 19970820. PRIORITY: US 1996-702767 19960822.

AB An advanced imaging spectrograph system includes an electrophoresis device, an optical imaging device, and a processor, configured to provide for slab-gel DNA sequencing and genotyping with high throughput sequencing. The system is based on

integration of improved electrophoresis structures with an imaging spectrophotometer that records the entire emission spectra along an imaging line across a sequencing gel (or capillary array). In one embodiment, the electrophoresis device includes a large number of

parallel

lanes formed in an electrophoresis gel which is sandwiched between two flat rectangular glass plates. The system includes spectral shape matching to improve dye identification allowing the use of dyes having nearly any emission spectra and allowing greater than four dye multiplexing.

IT 27072-45-3D, FITC, nucleotide conjugates

RL: ARU (Analytical role, unclassified); ANST (Analytical study) (as reporters in DNA sequencing; automatic DNA sequencer and genotyper

having extended spectral response)

RN 27072-45-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-5(or 6)-isothiocyanato- (9CI) (CA INDEX NAME)

$$D1-N=C=S$$

```
IC
     ICM G01N027-26
     ICS
         G01N027-447
     3-1 (Biochemical Genetics)
CC
     Section cross-reference(s): 9
ΙT
     Fluorescent dyes
        (as reporters in DNA sequencing; automatic DNA sequencer and
genotyper
        having extended spectral response)
     Spectrometers
IT
     Spectrometers
        (imaging; automatic DNA sequencer and genotyper having
        extended spectral response)
ΙT
     Optical imaging devices
       Optical imaging devices
        (spectrometers; automatic DNA sequencer and genotyper having
extended
        spectral response)
     27072-45-3D, FITC, nucleotide conjugates
                                                29270-56-2D, NBD-F,
ΙT
     nucleotide conjugates 82354-19-6D, Texas Red, nucleotide conjugates
     107347-53-5D, TRITC, nucleotide conjugates
     RL: ARU (Analytical role, unclassified); ANST (Analytical study)
        (as reporters in DNA sequencing; automatic DNA sequencer and
      . having extended spectral response)
    ANSWER 15 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN
1998:144771
              Document No. 128:155478 Convenient preparation of
fluorescein
                   Fujita, Satoshi; Nakanishi, Shingo; Toru, Takeshi
     derivatives.
     (Department of Applied Chemistry, Nagoya Institute of Technology,
     Showa-ku, Nagoya, 466, Japan). Synthetic Communications, 28(3),
387-393
     (English) 1998. CODEN: SYNCAV. ISSN: 0039-7911. Publisher: Marcel
     Dekker, Inc..
AB
     3'-O-Aralkyl-5-(4-biphenylcarboxamido)- and 3'-O-aralkyl-5-[N'-(3,5-
     dimethylphenyl)thioureido]fluorescein derivs. are prepared in high
yield by
     alkylation of 5-(4-biphenylcarboxamido) - and <math>5-[N'-(3,5-
     dimethylphenyl) thioureido] fluoresceins.
ΙT
     186187-60-0P 186187-63-3P 202747-86-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (convenient preparation of fluorescein derivs.)
     186187-60-0 HCAPLUS
RN
     [1,1'-Biphenyl]-4-carboxamide, N-[3'-[(3,4-dimethylphenyl)methoxy]-6'-
CN
     hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI)
(CA
     INDEX NAME)
```

RN 186187-63-3 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide,
N-[3'-hydroxy-6'-(1-naphthalenylmethoxy)-3oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)

CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic

Sensitizers)

IT 186187-60-0P 186187-63-3P 202747-86-2P

202747-87-3P 202747-88-4P 202747-89-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (convenient preparation of fluorescein derivs.)

L89 ANSWER 16 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 1997:663990 Document No. 127:343581 Detection of nucleic acids and proteins

using fluorescein derivative phosphate esters. Fujita, Satoshi;

Naoto; Momiyama, Masayoshi; Kondo, Yasumitsu; Nishiyauchi, Miho (Aisin Seiki Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 09262099 A2 19971007

Heisei, 14 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1996-74815

19960328.

GI

in

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Nucleic acids and proteins are detected by binding enzymes with the analytes, treating the labeled analytes with fluorescein derivative monophosphate esters, e.g., I, or diphosphate esters, e.g., II, and irradiating the resulting hydrolyzates with exciting light followed by detecting the emitted fluorescence. The method shows high sensitivity and

is applied for detecting DNA, RNA, proteins, nucleic acid-protein complexes, etc., in liquid samples, on a solid support, in cells, and

chromosomes. A nylon membrane was spotted with λDNA solns. of various concns., heated at 80° for 30 min, soaked in a solution of

<WALKE 10/789566><Page 98>

skim milk, and treated with alkaline phosphatase-labeled anti-digoxin $\ensuremath{\mathsf{Fab}}$

fragment. The film was further treated with a solution of I (preparation given)

in the dark at 37° for 1 h, followed by irradiation with UV light to detect fluorescence using a CCD camera. The detection limit was 5 fg.

IT 186187-57-5P 186187-60-0P 186187-63-3P 198074-76-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(nucleic acids and proteins detection using fluorescein derivative phosphate esters)

RN 186187-57-5 HCAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[3'-[(2,4-dimethylphenyl)methoxy]-6'-hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI)

(CA

INDEX NAME)

RN 186187-60-0 HCAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[3'-[(3,4-dimethylphenyl)methoxy]-6'-hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI)

(CA INDEX NAME)

RN 186187-63-3 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide,
N-[3'-hydroxy-6'-(1-naphthalenylmethoxy)-3oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)

```
RN 198074-76-9 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide,
N-[3'-hydroxy-6'-(2-naphthalenylmethoxy)-3-
oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)
```

IC ICM C12Q001-68

ICS G01N021-64; G01N021-78; G01N033-50; C12N015-09

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 3

IT 14002-51-8P, 4-Biphenylcarbonyl chloride 186187-55-3P

186187-57-5P 186187-60-0P 186187-63-3P

188007-59-2P 188007-84-3P **198074-76-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(nucleic acids and proteins detection using fluorescein derivative phosphate esters)

L89 ANSWER 17 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN 1997:338480 Document No. 127:29728 A novel fluorogenic substrate for the use

of nucleic acid hybridization. Fujita, Satoshi; Toru, Takeshi; Kondoh,

Yasumitsu; Momiyama, Masayoshi; Kagiyama, Naoto; Hori, Samuel H. (Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya,

466, Japan). Acta Histochemica et Cytochemica, 30(2), 165-172 (English)

1997. CODEN: ACHCBO. ISSN: 0044-5991. Publisher: Japan Society of Histochemistry and Cytochemistry.

AB The phosphates derived from newly synthesized 3'-O-aralkyl-5-(4-biphenylcarbox-amido) fluorescein derivs. were examined for the alkaline

phosphatase-linked fluorescence assay of the membrane-bound DNA. λ DNA was detectable to the amount of 5 fg in the assay using phosphorylated 5-(4-biphenylcarboxamido)-3'-0-(1-

 $\label{lem:naphthyl} \verb|naphthyl| \verb|methyl| fluorescein (BNFP). The spots gave distinguishably \\ \verb|clear|$

fluorescence without diffusion and nonspecific adsorption. In the

<WALKE 10/789566><Page 101>

Southern blot hybridization, 0.1 pg of DNA could be detected. Detection

of two different DNAs on a single blot was successfully performed by using

two different fluorogenic phosphates, Phosphrorylated N-(2-biphenyl)-3-

hydroxy-2-naphtalenecarboxamide (HNPP) and BNFP. The fluorescein derivs.

were also examined as substrates for horseradish peroxidase.

IT 190899-06-0P 190899-07-1P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST

(Analytical study); PREP (Preparation)

(novel fluorogenic substrate for use in nucleic acid hybridization)

RN 190899-06-0 HCAPLUS

CN Thiourea,

N-(3,5-dimethylphenyl)-N'-[3'-[(3,4-dimethylphenyl)methoxy]-6'hydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA

INDEX NAME)

Me
$$CH_2-O$$
 OH Me $NH-C-NH$

RN 190899-07-1 HCAPLUS

CN Thiourea,

N-(3,5-dimethylphenyl)-N'-[3'-hydroxy-6'-(1-naphthalenylmethoxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{HO} \\ \text{CH}_2 \\ \text{O} \\ \text{NH} \\ \text{C} \\ \text{NH} \\ \text{C} \\ \text{NH} \\ \text{O} \\ \text{O} \\ \end{array}$$

CC 3-1 (Biochemical Genetics)

Section cross-reference(s): 7

IT 186187-69-9P 186187-70-2P 186187-71-3P 188007-69-4P

190899-03-7P

190899-04-8P 190899-05-9P **190899-06-0P 190899-07-1P**

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST

(Analytical study); PREP (Preparation)

(novel fluorogenic substrate for use in nucleic acid hybridization)

L89 ANSWER 18 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1996:590758 Document No. 125:342530 Comparison of the photoelectric responses of monolayers of three fluorescein derivatives on SnO2 coated

substrate. Yuan, Feng; Bi, Zhi-chu; He, Jian-jun; Shen, Tao (Chinese Acad. of Sciences, Beijing, 100101, Peop. Rep. China). Dyes and Pigments,

32(1), 1-6 (English) 1996. CODEN: DYPIDX. ISSN: 0143-7208.

Publisher:

Elsevier.

AB Three types of fluorescein derivs. containing long alkyl chain(s) were synthesized and characterized. Their monolayers on a SnO2 coated substrate were fabricated, and their photoelec. responses evaluated.

IT 167314-71-8P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(synthesis of fluorescein derivs. with long alkyl chains and characterization of photoelec. responses of their monolayers on

SnO2

coated substrate)

RN 167314-71-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3'-(hexadecyloxy)-6'-hydroxy- (9CI) (CA INDEX NAME)

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

Section cross-reference(s): 76

IT 155556-88-0P **167314-71-8P** 167314-72-9P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(synthesis of fluorescein derivs. with long alkyl chains and characterization of photoelec. responses of their monolayers on

SnO2

coated substrate)

L89 ANSWER 19 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1994:545589 Document No. 121:145589 color filters. Furukawa, Tadahiro; Okamoto, Ryohei (Kyodo Printing Co Ltd, Japan). Jpn. Kokai Tokkyo Koho JP

06059114 A2 19940304 Heisei, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1992-233108 19920808.

AB A color filter comprises a heat-resistant resin containing ≥ 1 xanthene

dye, wherein the resin comprises a polyimide or a photosensitive acrylic polymer. The color filter is suited for use in high-definition

liquid-crystal display devices.

IT **6441-77-6**, Phloxine

RL: USES (Uses)

(heat-resistant color filters from, for liquid-crystal display devices)

RN 6441-77-6 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

2', 4', 5', 7'-tetrabromo-

4,7-dichloro-3',6'-dihydroxy-, dipotassium salt (9CI) (CA INDEX NAME)

●2 K

IC ICM G02B005-20

CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

Section cross-reference(s): 73

IT Dyes

(xanthene, heat-resistant color filters from, for liquid-crystal display

devices)

IT Optical imaging devices

(electrooptical liquid-crystal, heat-resistant color filters from)

IT 3520-42-1, Acid Rhodamine G 6441-77-6, Phloxine 9002-89-5,

Polyvinyl alcohol

RL: USES (Uses)

(heat-resistant color filters from, for liquid-crystal display devices)

L89 ANSWER 20 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1994:469651 Document No. 121:69651 Process for thermochemical generation of

generation or

acids for thermal imaging materials. Boggs, Roger A.; Grasshoff, Jurgen

M.; Mischke, Mark R.; Puttick, Anthony J.; Telfer, Stephen J.; Waller, David P.; Waterman, Kenneth C. (Polaroid Corp., USA). U.S. US 5278031 A

19940111, 19 pp. (English). CODEN: USXXAM. APPLICATION: US 1992-965172

19921023.

AB Certain squaric acid derivs. are useful for the thermochem. generation of

acids. The squaric acid derivs. may be used in thermal imaging materials

in conjunction with acid-sensitive materials which undergo a color change

when contacted by the acids generated from the squaric acid derivs. Preferably, the acid-sensitive materials undergo an irreversible color change, so that the images can be fixed by neutralizing all the acids generated with excess bases, thereby preventing further color change

in

the images during long term storage.

IT 70672-05-8

RL: USES (Uses)

(thermal printing materials containing squaric acid derivs. and)

RN 70672-05-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3'-hydroxy-6'-methoxy-

(9CI) (CA INDEX NAME)

IC ICM G03C005-16

NCL 430348000

CC 74-7 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 6674-22-2, 1,8-Diazabicyclo[5.4.0]undec-7-ene 70672-05-8

88878-49-3 104434-48-2 150773-00-5

RL: USES (Uses)

(thermal printing materials containing squaric acid derivs. and)

L89 ANSWER 21 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1993:90972 Document No. 118:90972 Optical imaging and apparatus therefor. Suzuki, Takayoshi (Kowa Co., Ltd., Japan). Jpn. Kokai Tokkyo

Koho JP 04184209 A2 19920701 Heisei, 9 pp. (Japanese). CODEN: JKXXAF.

APPLICATION: JP 1990-312925 19901120.

AB The title method comprises (1) incidence of a coherent probe light which

<WALKE 10/789566><Page 106>

has an optical image corresponding to an initial shape of the object and a

coherent pumping light coherently into a film containing an organic dye

for recording of the optical image from the object as irreversible hologram in the film, and (2) incidence of a probe light having a current

image of the object into the film and 2 pumping light having direction of

polarization vertical to the probe light into the film from the both sides

for generation of 2 phase-conjugate waves, passage thereof through a polarization plate in the direction such that the amplitudes of the waves

cancel to each other, and production of optical signals corresponding to a

difference between the optical imanes of the initial and the current shape

of the object.

IT **16423-68-0**, Erythrosine B

RL: USES (Uses)

(optical imaging by holog.-phase conjugate wave generation with film containing)

RN 16423-68-0 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-2',4',5',7'-tetraiodo-, disodium salt (9CI) (CA INDEX NAME)

●2 Na

IC ICM G01B011-16

ICS G01B009-027; G01B011-24; G02F001-35; G03H001-04

CC 74-8 (Radiation Chemistry, Photochemistry, and Photographic and Other

Reprographic Processes)

Section cross-reference(s): 73

- ST holog imaging org dye film; phase conjugate wave optical imaging
- IT Holography

(optical imaging by phase conjugate wave generation from organic dye-containing film with)

IT Dyes

(organic, films containing, for optical **imaging** by holog.-phase conjugate wave generation)

IT Optical imaging devices

(real time holog.-phase conjugate wave generation, with organic dye-containing films)

IT 16423-68-0, Erythrosine B

RL: USES (Uses)

(optical imaging by holog.-phase conjugate wave generation with film containing)

L89 ANSWER 22 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1991:404720 Document No. 115:4720 Enzyme assay method using an enzyme amplification system. Abuknesha, Ramadan Arabi; Bennetto, Hugh Peter; Mason, Jeremy Richard; Nugent, Philip Giles; Stirling, John Laing; Thurston, Christopher Frank (Alcan International Ltd., Can.). Eur.

Pat.

Appl. EP 313274 A1 19890426, 19 pp. DESIGNATED STATES: R: BE, CH, DE,

ES, FR, GB, IT, LI, NL, SE. (English). CODEN: EPXXDW. APPLICATION:

1988-309624 19881014. PRIORITY: GB 1987-24764 19871022.

AB An immunoassay method involves the use of 1 or preferably 2 enzyme amplification steps to increase assay speed or sensitivity. In a 1st step, a 1st enzyme is generated in an amount related to the concentration of an

analyte in a sample. In a 2nd step, the 1st enzyme acts on a 1st substrate to reveal antigenic determinants of a 1st product. In a 3rd step, the 1st product is reacted with an antibody. The extent of this immune reaction is determined, preferably by means of an enzyme signal system.

A nonimmunochem. assay system using the above enzyme amplification is also

described. An ouabain-fetuin conjugate (preparation described) was immobilized

on microtiter plate wells, to which were added $\beta\text{-galactosidase-conjugated}$ anti-digoxin IgG. Digoxin was added to the wells, and after 1

h at 37°, the contents were transferred to plates containing immobilized bovine serum albumin-coumarin- β -galactoside conjugate. After 2 h at 37°, alkaline phosphatase-conjugated anti-coumarin IgG was

added to each well, and after 1.5 h at 37°, the plates were washed and alkaline phosphatase substrate was added. Absorbance was read at 410 nm,

and bound alkaline phosphatase activity was proportional to the digoxin concentration

IT 134240-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and reaction of, for enzyme amplification enzyme immunoassay)

RN 134240-32-7 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3'-hydroxy-6'-methoxy-

5(or 6)-nitro- (9CI) (CA INDEX NAME)

 $D1-NO_2$

IC ICM G01N033-58

ICS G01N033-543; G01N033-74; G01N033-533

ICA G01N033-94

CC 9-10 (Biochemical Methods)

Section cross-reference(s): 25, 80

IT 134240-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and reaction of, for enzyme amplification enzyme immunoassay)

L89 ANSWER 23 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1990:517056 Document No. 113:117056 Spectrophotometric determination of ionization and isomerization constants of Rose Bengal, Eosin Y and some

<WALKE 10/789566><Page 109>

derivatives. Amat-Guerri, F.; Lopez-Gonzalez, M. M. C.; Sastre, R.; Martinez-Utrilla, R. (Inst. Quim. Org., CSIC, Madrid, 28006, Spain). Dyes

and Pigments, 13(3), 219-32 (English) 1990. CODEN: DYPIDX. ISSN: 0143-7208.

AB The exptl. pK values corresponding to the acid forms of Rose Bengal (I),

Eosin Y (II), their Me esters, their Me ethers, and the decarboxylated compound derived from I, all of them in solution in 1:1 mixts. of dioxane with

aqueous buffers, were determined by applying graphical methods to visible

spectrophotometric data. Assuming the same visible absorption spectra for $% \left(1\right) =\left(1\right) +\left(1\right) +$

mols. with similar chromophoric groups, the isomerization consts. of the

possible equilibrium between lactonic and quinonoid tautomeric structures, and

the pK values of the ionizations of the mol. forms which could be present,

were estimated In the quinonoid mol. forms of I and II, their phenol groups

were ionized first, with estimated pK values of 2.57 and 2.69, resp., while

their carboxylic groups showed much less acidity, and pK values of 5.01

and 6.25.

IT 118584-84-2 127424-66-2

RL: USES (Uses)

(ionization and tautomerization consts. of, determination of, spectrophotometric)

RN 118584-84-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

4,5,6,7-tetrachloro-3'-

hydroxy-2',4',5',7'-tetraiodo-6'-methoxy- (9CI) (CA INDEX NAME)

RN 127424-66-2 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,
2',4',5',7'-tetrabromo-6'hydroxy-3'-methoxy- (9CI) (CA INDEX NAME)

 ${\tt CC}$ 41-8 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic

Sensitizers)

IT 106805-50-9 115546-28-6 **118584-84-2 127424-66-2**

127424-70-8 127424-71-9 127424-74-2

RL: USES (Uses)

(ionization and tautomerization consts. of, determination of, spectrophotometric)

L89 ANSWER 24 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN
1990:45806 Document No. 112:45806 Optical information multiple-recording
materials using fluorescein. Sakota, Kazuaki; Kominami, Kazuhiko;
Iwamoto, Masao (Agency of Industrial Sciences and Technology, Japan).
Jpn. Kokai Tokkyo Koho JP 01152452 A2 19890614 Heisei, 4 pp.
(Japanese).

CODEN: JKXXAF. APPLICATION: JP 1987-309450 19871209.

Ι

GΙ

AB The title recording materials are composed of (1) fluorescein derivs. of

the formula I (M = alkaline metal; R = alkaline metal, alkyl) as a quest component

and (2) a polymer as a host component, which can dissolve the guest component; the guest component used may be fluorescein di-Na salt, methoxyfluorescein Na salt, or ethoxyfluorescein Na salt, and the host component may be poly(vinyl alc.). The recording materials, which use the

photochem. hole burning (PHB) phenomenon, show excellent heat stability.

Thus, fluorescein di-Na salt was dissolved in aqueous poly(vinyl alc.), then

made into a film having a guest concentration of 10-2 mol/L and a thickness of

0.5 mm. The film was cooled to liquid He temperature, and irradiated with a $496.4\,$

 $\,$ nm laser beam to form a PHB hole, and, after elevating the temperature, the film

showed good PHB hole recovery.

IT 124591-82-8 124591-83-9

RL: USES (Uses)

(photochem. hole burning optical recording material containing guest

component from, with heat stability)

RN 124591-82-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3'-hydroxy-6'-methoxy-,

sodium salt (9CI) (CA INDEX NAME)

Na

Na

IC ICM G03C001-72

ICS G11B007-24 C07D311-80; G06K019-00

IT 518-47-8, Fluorescein disodium salt 124591-82-8

124591-83-9

guest

RL: USES (Uses)

(photochem. hole burning optical recording material containing

component from, with heat stability)

L89 ANSWER 25 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1989:57461 Document No. 110:57461 General synthesis of new Rose Bengal derivatives with ether functional groups. Xu, Danian; Vanloon, Adriaan;

Linden, Shwn Meei; Neckers, D. C. (Cent. Photochem. Sci., Bowling Green

State Univ., Bowling Green, OH, 43403, USA). Journal of Photochemistry,

38, 357-63 (English) 1987. CODEN: JPCMAE. ISSN: 0047-2670.

AB Functionalization at the C-2' and C-6 positions of benzopyran I was described. Derivs. obtained included the C-2' ester, C-6 ether, C-6 Na

salt, and the C-2' Na salt/C-6 ether.

IT 118584-84-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and reactions of)

RN 118584-84-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

4, 5, 6, 7-tetrachloro-3'-

hydroxy-2',4',5',7'-tetraiodo-6'-methoxy- (9CI) (CA INDEX NAME)

CC 27-14 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 41

IT 118584-84-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
 (preparation and reactions of)

L89 ANSWER 26 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1986:456924 Document No. 105:56924 Characterization of ouabain-sensitive phosphatase activity in the absence of potassium ion in purified pig kidney sodium-potassium ATPase. Nagamune, Hideaki; Urayama, Osamu; Hara,

Yukichi; Nakao, Makoto (Sch. Med., Tokyo Med. Dent. Univ., Tokyo, 113, Japan). Journal of Biochemistry (Tokyo, Japan), 99(6), 1613-24 (English)

1986. CODEN: JOBIAO. ISSN: 0021-924X.

AB The ouabain-sensitive phosphatase activity of purified pig kidney Na,K-ATPase preparation in the absence of K+ ((-K)phosphatase) was examined

precisely. During the preparation procedures, the (-K)3-O-methylfluoresceinphosphatase [(-K)3-OMFPase] activity or the (-K)p-nitrophenylphosphatase [(-K)pNPPase] activity appeared to be purified in parallel with the Na,K-ATPase activity. The (-K)phosphatase

activity was competitively inhibited by ATP and by ADP, with Ki vales of

0.25 and 1.4 $\mu M\text{,}$ resp. These values are consistent with their dissociation

consts. for the high-affinity ATP-binding site of the Na,K-ATPase. The

substrate, pNPP, apparently competed with covalently bound FITC, which is

known to bind in the neighborhood of the high-affinity ATP-binding site of

the Na,K-ATPase, in both the (-K)phosphatase and the (+K)phosphatase reactions. The FITC-fluorescence intensity of FITC-labeled enzyme at the

maximal steady-state activity of the (-K)phosphatase reaction was at a similar level to that of the enzyme E2 species. However, the FITC-labeled

enzyme in the presence of only Mg2+ or only pNPP gave a fluorescence level $% \left(1\right) =\left(1\right) +\left(1\right)$

similar to that of the enzyme El species. Oligomycin inhibited the (-K)phosphatasè activity by ≤46%. Apparently the (-K)phosphatase reaction is catalyzed at the high-affinity ATP-binding site of Na,K-ATPase, and the (-K)phosphatase reaction proceeds in a cyclic manner

 $(E1\rightarrow E2\rightarrow E1)$.

IT 70672-05-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ouabain-sensitive phosphatase of kidney ATPase, kinetics of)

RN 70672-05-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3'-hydroxy-6'-methoxy-

(9CI) (CA INDEX NAME)

CC 7-4 (Enzymes)

IT 70672-05-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ouabain-sensitive phosphatase of kidney ATPase,
kinetics of)

L89 ANSWER 27 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1985:42494 Document No. 102:42494 Methods and structures employing non-radioactive chemically-labeled polynucleotide probes.
Stavrianopoulos, Jannis G.; Kirtikar, Dollie; Johnston, Kenneth H.; Thalenfeld, Barbara E. (Enzo Bio Chem, Inc., USA). Eur. Pat. Appl. EP

<WALKE 10/789566><Page 116>

117440 A1 19840905, 76 pp. DESIGNATED STATES: R: AT, BE, CH, DE, FR, GB,

IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1984-100836 19840126. PRIORITY: US 1983-461469 19830127.

AB The title probes, such as single-stranded DNA probes containing ≥ 25 bases, contain especially enzyme labels and are used for the detection and

identification of complementary single-stranded DNA (fixed on an inert support) by hybridization, followed by spectrophotometric determination of the

enzyme in the double-stranded hybrids formed. These probes can replace

hazardous, expensive, short-lived radiolabeled probes, and ELISA also can

be used to determine the formed hybrid. The support may be glass, polystyrene,

nitrocellulose, dextran, etc. Recommended enzyme labels and some substrates are tabulated. The method is useful for detecting the presence

of pathogens (e.g., Streptococcus, Staphylococcus, Pneumococcus, etc.) in

clin. samples by detection of their genetic material.

IT 70672-05-8

RL: ANST (Analytical study)

(as acid phosphatase substrate, in DNA hybridization tests)

RN 70672-05-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3'-hydroxy-6'-methoxy-

(9CI) (CA INDEX NAME)

IC C07H021-00; G01N033-58

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 15

IT 4264-83-9 23915-89-1 51379-07-8 **70672-05-8**

RL: ANST (Analytical study)

(as acid phosphatase substrate, in DNA hybridization tests)

<WALKE 10/789566><Page 117>

L89 ANSWER 28 OF 28 HCAPLUS COPYRIGHT 2004 ACS on STN

1982:3192 Document No. 96:3192 Preparation and spectral properties of lipophilic fluorescein derivatives: application to plasma low-density lipoprotein. Falck, J. R.; Krieger, Monty; Goldstein, J. L.; Brown, M. S.

(Health Sci. Cent., Univ. Texas, Dallas, TX, 75235, USA). Journal of the

American Chemical Society, 103(24), 7396-8 (English) 1981. CODEN: JACSAT.

ISSN: 0002-7863.

AB The preparation of several fluorescein derivs., specifically designed for

reconstitution into low-d. lipoprotein (LDL), and esterified with cholesteryl ricinoleate is described. Their spectral properties are compared with fluorescein. The esters are .apprx.40-50-fold more fluorescent than the corresponding acids and fluorescein in 5% HOAC/ETOH.

As a consequence of their unique structure and fluorescence characteristics, these probes are valuable tools in the study of LDL and

cholesterol metabolism

IT 70672-05-8

RL: RCT (Reactant); RACT (Reactant or reagent) (esterification of, with cholesteryl ricinoleate)

RN 70672-05-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one,

3'-hydroxy-6'-methoxy-

(9CI) (CA INDEX NAME)

CC 9-5 (Biochemical Methods)

IT 3348-03-6 **70672-05-8** 79955-27-4

RL: RCT (Reactant); RACT (Reactant or reagent) (esterification of, with cholesteryl ricinoleate)

 \Rightarrow \Rightarrow d 183 1-21 cbib abs hitstr hitind

L83 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN 2004:207656 Document No. 140:392329 Synthesis and characterization of zinc

sensors based on a monosubstituted fluorescein platform. Nolan, Elizabeth

M.; Burdette, Shawn C.; Harvey, Jessica H.; Hilderbrand, Scott A.; Lippard, Stephen J. (Department of Chemistry, Massachusetts Institute of

Technology, Cambridge, MA, 02139, USA). Inorganic Chemistry, 43(8), 2624-2635 (English) 2004. CODEN: INOCAJ. ISSN: 0020-1669. Publisher:

American Chemical Society.

AB The synthesis of a new fluorescein carboxaldehyde asym. substituted on the

xanthene (top) ring is reported. This mol. is a key precursor for two of

three monofunctionally derivatized fluorescein-based Zn(II) sensors presented in this work. Detailed preparative routes to, and photophys.

characterization of, these sensors are described. The sensors are based

on the previously reported ${\ensuremath{\mathtt{ZP4}}}$ motif by the authors (2003) and incorporate

a di(2-picolyl)amine-containing aniline-derivatized ligand framework. By

varying the nature of the substituent para to the aniline nitrogen atom,

which is responsible for photoinduced electron transfer quenching the unbound ZP dye, we investigated the extent to which such electronic tuning might improve the fluorescent properties of asym. ZP sensors. Although a comparison of probes with X = H, F, Cl, OMe reveals

that the photophys. behavior of these **dyes** is not readily predictable, our methodol. illustrates the ease with which aniline-based.

ligands may be linked to fluorescein dyes.

IT 389625-48-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of zinc sensors based on monosubstituted fluorescein platform)

RN 389625-48-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

2'-chloro-3',6'-dihydroxy-

5'-methyl- (9CI) (CA INDEX NAME)

 ${\it CC}$ 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic

Sensitizers)

Section cross-reference(s): 9, 27, 73, 80

ST zinc sensor fluorescein dye deriv prepn

IT 389625-41-6P 502467-23-4P 686767-89-5P 686767-90-8P RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (dye; preparation of zinc sensors based on monosubstituted

fluorescein platform)

TT 77-48-5, 1,3-Dibromo-5,5-dimethylhydantoin 446-33-3, 5-Fluoro-2-nitrotoluene 1539-42-0, Bis(2-picolyl)amine 389625-48-3 389625-50-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of zinc sensors based on monosubstituted fluorescein platform)

L83 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN 2003:221905 Document No. 138:256581 Fluorescent dyes and their production for fluorescent labeling of biomolecules. Lukhtanov, Eugeny

A.; Vorobiev, Alexei V.; Reed, Michael W.; Vermeulen, Nicolaas M. J. (Epoch Biosciences, Inc., USA). PCT Int. Appl. WO 2003023357 A2 20030320,

103 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG,

BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI,

GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ,

LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM,

PH, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,

UG,
US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM;
RW:

<WALKE 10/789566><Page 120>

AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR,

IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-US28543 20020906. PRIORITY: US 2001-PV317875 20010907; US 2001-26374 20011221.

AB Xanthene, benzoxanthene, phenothiazine, benzophenothiazine, and coumarin

lactone dye reagents useful in labeling biol. materials are provided along with methods for their use. The dyes are suitable for multiple detection processes and may be readily converted to

reactive yet stable labeling reagents. In example,

8,12,23,24-tetrachloro-

9-hydroxy-10-methylspiro[3,4-dihydro-2H-pyrano[3,2-b]xanthene-6,3'-3-hydroisobenzofuran]-2,19-dione was prepared and condensed with 6-aminohexanol and 2-cyanoethyl N,N-diisopropylchlorophosphoramidite

give a fluorescent labeling reagent.

IT 502484-48-2P 502484-52-8P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material

use); PREP (Preparation); USES (Uses)

(dye; production of fluorescent dyes for fluorescent labeling of biomols.)

RN 502484-48-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2'-propanoic acid, 4,4',7,7'-tetrachloro-3',6'-dihydroxy-5'-methyl-3-oxo- (9CI) (CFINDEX

NAME)

to

HO OH
$$C1$$
 $CH_2-CH_2-CO_2H$

RN 502484-52-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2'-propanoic acid, 4',5,6,7'-tetrachloro-3',6'-dihydroxy-5'-methyl-3-oxo- (9CI) (CA INDEX

NAME)

$$\begin{array}{c} \text{Me} & \text{Cl} \\ \text{HO} & \text{OH} \\ \text{Cl} & \text{CH}_2-\text{CH}_2-\text{CO}_2\text{H} \\ \text{Cl} & \text{O} \end{array}$$

IT 502485-30-5P 502485-35-0P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);

RACT

(Reactant or reagent)

(intermediate; production of fluorescent **dyes** for fluorescent

labeling of biomols.)

RN 502485-30-5 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4'-propanoic acid,

2',5,6,7'-tetrachloro-3',6'-dihydroxy-5'-methyl-3-oxo- (9CI) (CA

INDEX

NAME)

$$HO_2C-CH_2-CH_2$$
 Me
 HO OH
 $C1$ C1

RN 502485-35-0 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2'-propanamide,

N-[6-[bis(4-methoxyphenyl)phenylmethoxy]hexyl]-4',5,6,7'-tetrachloro-3',6'-dihydroxy-5'-methyl-3-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{HO} \\ \text{Cl} \\ \text{Cl} \\ \text{Cl} \\ \text{O} \\ \text{OH} \\ \text{CH}_2-\text{CH}_2-\text{C-NH-} \text{(CH}_2) 6-\text{O-C} \\ \text{Ph} \\ \text{Cl} \\ \text{O} \\ \text{OMe} \\ \text{OH}_2-\text{CH}_2-\text{C-NH-} \text{(CH}_2) 6-\text{O-C} \\ \text{OH}_2-\text{C-NH-} \\ \text{OH}_2-\text{C-NH-}$$

IT 502485-33-8

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; production of fluorescent dyes for fluorescent labeling of biomols.)

RN 502485-33-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2'-propanamide,

4',5,6,7'-tetrachloro-3',6'-dihydroxy-N-(6-hydroxyhexyl)-5'-methyl-3-oxo-(9CI) (CA INDEX NAME)

IC ICM G01N

CC $\,$ 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic $\,$

Sensitizers)

Section cross-reference(s): 9, 27, 28

ST fluorescent dye prodn labeling biomol

IT Fluorescent dyes

Fluorescent indicators

502484-73-3P

```
(production of fluorescent dyes for fluorescent labeling of
        biomols.)
     502484-45-9P
                    502484-46-0P
                                   502484-47-1P
                                                   502484-59-5P
502484-67-5P
     RL: IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or
     engineered material use); PREP (Preparation); RACT (Reactant or
reagent);
     USES (Uses)
        (dye; production of fluorescent dyes for fluorescent
        labeling of biomols.)
     502484-05-1P
                    502484-06-2P
                                   502484-38-0P
                                                   502484-39-1P
502484-40-4P
     502484-41-5P
                    502484-42-6P
                                   502484-43-7P
                                                   502484-44-8P
     502484-48-2P
                    502484-49-3P
                                   502484-50-6P
                                                   502484-51-7P
                    502484-53-9P
                                   502484-54-0P
     502484-52-8P
                                                   502484-60-8P
     502484-61-9P
                    502484-62-0P
                                   502484-63-1P
                                                  502484-64-2P
502484-65-3P
     502484-69-7P
                    502484-76-6P
                                   502484-78-8P
                                                   502484-82-4P
502484-86-8P
                    502484-90-4P
     502484-88-0P
                                   502484-92-6P
                                                  502484-94-8P
502484-96-0P
     502484-98-2P
                    502485-00-9P
                                   502485-02-1P
                                                   502485-04-3P
502485-06-5P
     502485-08-7P
                    502485-18-9P
                                   502485-20-3P
                                                  502485-32-7P
502485-39-4P
     RL: IMF (Industrial manufacture); TEM (Technical or engineered
material
     use); PREP (Preparation); USES (Uses)
        (dye; production of fluorescent dyes for fluorescent
        labeling of biomols.)
     502483-92-3P
                    502483-93-4P
                                   502483-94-5P
                                                   502483-95-6P
502483-96-7P
     502483-97-8P
                    502483-98-9P
                                   502483-99-0P
                                                   502484-00-6P
502484-01-7P
                                   502484-04-0P
     502484-02-8P
                    502484-03-9P
                                                  502484-07-3P
502484-08-4P
     502484-09-5P
                    502484-10-8P
                                   502484-11-9P
                                                   502484-12-0P
502484-13-1P
                    502484-15-3P
                                   502484-16-4P
                                                   502484-17-5P
     502484-14-2P
502484-18-6P
     502484-19-7P
                    502484-20-0P
                                   502484-21-1P
                                                   502484-22-2P
502484-23-3P
     502484-24-4P
                    502484-25-5P
                                   502484-26-6P
                                                   502484-27-7P
502484-29-9P
                    502484-31-3P
                                   502484-32-4P
     502484-30-2P
                                                   502484-33-5P
502484-34-6P
     502484-35-7P
                    502484-36-8P
                                   502484-37-9P
                                                   502484-71-1P
```

<WALKE 10/789566><Page 124>

```
502484-80-2P
                    502485-12-3P 502485-14-5P
                                                  502485-16-7P
502485-24-7P
     502485-26-9P 502485-30-5P 502485-35-0P
                                              502485-37-2P
     RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);
RACT
     (Reactant or reagent)
        (intermediate; production of fluorescent dyes for fluorescent
        labeling of biomols.)
                    502484-56-2P
                                                  502484-58-4P
     502484-55-1P
                                   502484-57-3P
ΙT
     RL: IMF (Industrial manufacture); TEM (Technical or engineered
material
     use); PREP (Preparation); USES (Uses)
        (intermediate; production of fluorescent dyes for fluorescent
        labeling of biomols.)
     67-56-1, Methanol, reactions 95-88-5, 4-Chlororesorcinol
ΙT
                                                                  117-08-8.
     Tetrachlorophthalic anhydride 128-09-6, N-Chlorosuccinimide
132-86-5,
     1,3-Dihydroxynaphthalene 141-82-2, Malonic acid, reactions
575-44-0,
     1,6-Dihydroxynaphthalene
                               674-82-8, Diketene 698-31-7,
     4-Nitrosoresorcinol 942-06-3, 4,5-Dichlorophthalic anhydride
     1538-75-6, Trimethylacetic anhydride
                                           4048-33-3, 6-Aminohexanol
                               89992-70-1, 2-Cyanoethyl N, N-
     17422-90-1
                  72482-14-5
     diisopropylchlorophosphoramidite
                                      502483-90-1 502483-91-2
502484-84-6
                   502485-22-5
     502485-10-1
                                 502485-28-1 502485-33-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (starting material; production of fluorescent dyes for
        fluorescent labeling of biomols.)
L83
   ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
            Document No. 138:353859 Solvent-free synthesis of
2003:4189
     sulfonephthaleins, sulfonefluoresceins and fluoresceins under
microwave
     irradiation. Cihelnik, Simon; Stibor, Ivan; Lhotak, Pavel
(Department of
     Organic Chemistry, Institute of Chemical Technology, Prague, Prague,
166
     28, Czech Rep.). Collection of Czechoslovak Chemical Communications,
     67(12), 1779-1789 (English) 2002. CODEN: CCCCAK. ISSN: 0010-0765.
OTHER
     SOURCES: CASREACT 138:353859. Publisher: Institute of Organic
Chemistry
     and Biochemistry, Academy of Sciences of the Czech Republic.
     The title compds. are prepared from phenols and 2-sulfobenzoic
AΒ
anhydride or
     phthalic anhydride under microwave irradiation
IT
     118797-71-0P
```

RL: SPN (Synthetic preparation); PREP (Preparation) (solvent-free synthesis of sulfonephthaleins, sulfonefluoresceins

fluoresceins from phenols and 2-sulfobenzoic anhydride or phthalic anhydride under microwave irradiation)

RN 118797-71-0 HCAPLUS

Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, CN

3',6'-dihydroxy-4',5'-

dimethyl- (9CI) (CA INDEX NAME)

CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))

ΙT Dyes

and

(solvent-free synthesis of sulfonephthaleins, sulfonefluoresceins and

> fluoresceins from phenols and 2-sulfobenzoic anhydride or phthalic anhydride under microwave irradiation)

115-41-3P, Pyrocatechol violet 125-31-5P, p-Xylenol blue 143-74-8P,

Phenol red 1733-12-6P, o-Cresol red 2103-64-2P, Gallein .2303-01-7P,

2321-07-5P, Fluorescein 4424-03-7P, m-Cresol purple Sulfonefluorescein

32638-88-3P, Pyrogallol red

78512-32-0P 118797-71-0P 518979-55-0P, 122079-34-9P 216771-46-9P

2,6-Xylenolsulfonephthalein

518979-56-1P, Methylsulfonefluorescein 518979-57-2P 590409-46-4P RL: SPN (Synthetic preparation); PREP (Preparation)

(solvent-free synthesis of sulfonephthaleins, sulfonefluoresceins

and

fluoresceins from phenols and 2-sulfobenzoic anhydride or phthalic anhydride under microwave irradiation)

L83 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN 2002:51568 Document No. 136:103838 Fluorescein-based metal sensors and their

<WALKE 10/789566><Page 126>

```
Lippard, Stephen J.; Burdette, Shawn; Hilderbrand, Scott; Tsien,
     Roger; Walkup, Grant (Massachusetts Institute of Technology, USA).
PCT
     Int. Appl. WO 2002004562 A2 20020117, 98 pp. DESIGNATED STATES: W:
AE,
     AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR,
CU,
     CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,
IL,
     IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
MG,
    MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
TJ,
     TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
MD,
     RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES,
FI,
     FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG,
TR.
     (English). CODEN: PIXXD2. APPLICATION: WO 2001-US41313 20010709.
     PRIORITY: US 2000-PV216872 20000707; US 2000-PV216875 20000707; US
     2001-PV284384 20010417.
AΒ
     Fluorescein-based ligands are obtained for the detection of metal
ions,
     such as zinc in intracellular media. In an example, an orange dye
     was produced by reductive amination of
4',5'-fluoresceindicarboxaldehyde
     with bis(2-pyridylmethyl)amine and shown to have a Zn-selective
     fluorescence response.
ΙΤ
     389625-48-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (starting material; preparation and crystal structure of
fluorescein-based
        ligand-zinc complex)
     389625-48-3 HCAPLUS
RN
     Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,
2'-chloro-3', 6'-dihydroxy-
     5'-methyl- (9CI) (CA INDEX NAME)
```

IT 118797-71-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; production of fluorescein-based metal sensors selective

for zinc)

RN 118797-71-0 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3',6'-dihydroxy-4',5'-

dimethyl- (9CI) (CA INDEX NAME)

IC ICM C09B011-08

ICS G01N033-533; G01N033-58

CC 41-11 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic

Sensitizers)

Section cross-reference(s): 9, 27, 78, 79, 80

ST fluorescein based dye prodn zinc fluorescent sensor

intracellular

IT 389625-18-7P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material \cdot

```
use); PREP (Preparation); USES (Uses)
        (dye; production of fluorescein-based metal sensors selective for
        zinc)
     357916-12-2P
IT
     RL: IMF (Industrial manufacture); TEM (Technical or engineered
material
     use); PREP (Preparation); USES (Uses)
        (orange dye; production of fluorescein-based metal sensors and
        their use)
ΙT
     389625-25-6P
     RL: IMF (Industrial manufacture); TEM (Technical or engineered
material
     use); PREP (Preparation); USES (Uses)
        (orange dye; production of fluorescein-based metal sensors
        selective for zinc)
     288574-78-7P
ΙT
     RL: IMF (Industrial manufacture); TEM (Technical or engineered
material
     use); PREP (Preparation); USES (Uses)
        (salmon pink dye; production of fluorescein-based metal sensors
        selective for zinc)
ΙT
     1333-74-0, Hydrogen, reactions 5367-32-8, 3-Methyl-4-nitroanisole
     389625-48-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (starting material; preparation and crystal structure of
fluorescein-based
        ligand-zinc complex)
     62-53-3, Aniline, reactions 127-08-2, Potassium acetate
ΙT
                                                                 127-09-3,
     Sodium acetate
                      699-83-2 2321-07-5, Fluorescein
                                                          2491-18-1,
     L-Methionine methyl ester hydrochloride 2706-56-1, 2-(2-
     Aminoethyl)pyridine 6201-65-6, 2-Chlororesorcinol 7335-65-1,
Hydrazine
               7761-88-8, Silver nitrate, reactions
                                                      13154-24-0,
     acetate
     Triisopropylsilyl chloride 18162-48-6, tert-Butyldimethylsilyl
chloride
     30525-89-4, Paraformaldehyde 58479-61-1, tert-Butyldiphenylsilyl
     chloride 65840-40-6, Potassium levulinate 118797-71-0
     389625-23-4
                   389625-31-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (starting material; production of fluorescein-based metal sensors
selective
        for zinc)
     389625-47-2P
IT
     RL: IMF (Industrial manufacture); PREP (Preparation)
        (yellow dye; preparation and crystal structure of
        fluorescein-based ligand-zinc complex)
                    389625-26-7P
     389625-19-8P
                                   389625-27-8P
     RL: IMF (Industrial manufacture); TEM (Technical or engineered
material
```

<WALKE 10/789566><Page 129>

use); PREP (Preparation); USES (Uses)
 (yellow dye; production of fluorescein-based metal sensors
 selective for zinc)

L83 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN 1995:790946 Document No. 123:301216 Sensitivity enhancement of fluorescent

pH indicators using pH-dependent energy transfer. Gabor, Gabriella; Chadha, Suneet; Walt, David R. (Max Tishler Laboratory for Organic Chemistry, Department of Chemistry, Tufts University, 62 Talbot Ave., Medford, MA, 02155, USA). Analytica Chimica Acta, 313(1-2), 131-7 (English) 1995. CODEN: ACACAM. ISSN: 0003-2670. Publisher:

Elsevier.

The

AB The concept of energy transfer is examined, in view of its application to

enhance pH sensitivity of fluorescent **dyes**. Two fluorescent pH sensitive indicators are chosen such that they have nearly the same pKa

values and have maximum spectral overlap between the emission spectrum of the

donor and the excitation spectrum of the acceptor. In this work we studied the pH dependent energy transfer between 7-hydroxy-4-methylcoumarin-3-acetic acid (HCA) as the donor with fluorescein and 5-(and 6-)carboxy-4',5'-dimethyl fluorescein (CDF) as the acceptors.

extent of energy transfer was measured exptl. by following the increase in

acceptor emission at different pH values. The sensitivity of the acceptor

dye is almost double when excited via energy transfer, provided the donor emission itself exhibits a similar dependence on pH. The pF sensitivity of fluorescein (Δ I/ Δ pH), was observed to increase from 0.28 when excited directly, to 0.71 when excited via energy transfer.

CDF also shows a similar increase from 0.49 to 0.71.

IT 100111-02-2, 5-Carboxy-4',5'-dimethyl fluorescein

100111-03-3, 6-Carboxy-4',5'-dimethyl fluorescein

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(sensitivity enhancement of fluorescent pH indicators using pH-dependent energy transfer)

RN 100111-02-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

RN 100111-03-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

Section cross-reference(s): 73, 79, 80

ST fluorescent dye pH indicator energy transfer

IT Dyes

Indicators

(fluorescent, sensitivity enhancement of fluorescent pH indicators using pH-dependent energy transfer)

IT 2321-07-5, Fluorescein 2747-05-9, 7-Hydroxy-4-methylcoumarin acetate 100111-02-2, 5-Carboxy-4',5'-dimethyl fluorescein

100111-03-3, 6-Carboxy-4',5'-dimethyl fluorescein

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(sensitivity enhancement of fluorescent pH indicators using pH-dependent energy transfer)

<WALKE 10/789566><Page 131>

L83 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
1995:199694 Document No. 122:4777 Free concentrations of intracellular
fluorescent anions determined by cytoplasmic dialysis of isolated
hepatocytes. Weinman, Steven A.; Maglova, Lilia M. (Dep. Internal
Med.,

Univ. Texas Med. Branch, Galveston, TX, 77555-0641, USA). American Journal of Physiology, 267(5, Pt. 1), G922-G931 (English) 1994. CODEN:

AJPHAP. ISSN: 0002-9513. Publisher: American Physiological Society. AB Intracellular organic ions exist in free solution bound to cytoplasmic proteins,

partitioned within intracellular membranes, and enclosed in intracellular

vesicles and organelles. The aim of this study was to develop a $\operatorname{\mathsf{method}}$

accomplished by measuring initial rates of diffusion between patch-clamp

pipets and cell cytoplasm and determining the null-point concentration of this process.

Carboxydimethylfluorescein (CF) was used as a model compound It readily

diffused between cytoplasm and pipet, and there was a linear relationship

between concentration in the pipet and equilibrium cell fluorescence. When cells

previously loaded with CF were patched, intracellular fluorescence rapidly

changed in a pos. or a neg. direction, depending on the concentration of CF in

the pipet. The null point, defined as the concentration at which cells neither

gained nor lost fluorescence, described the same relationship between free

concentration and total cell fluorescence as that determined by direct loading of the

cells to equilibrium In hepatocytes preloaded with a fluorescent bile acid

derivative, cholylglycylamidofluorescein (CGamF), by exposure (0.05 μ M) for

 $^{\circ}$ 30 min, the null point occurred at a CGamF concentration in the pipet of 0.6

 $\mu M.$ This value is 12 times greater than that in the bath. A new method is described that can measure free cytosolic concns. of fluorescent

mols. It should prove useful in determining the intracellular location and

state of transported organic ions.

IT 103991-76-0

RL: ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process)

(intracellular fluorescent anions determination by cytoplasmic dialysis of

hepatocytes)

RN 103991-76-0 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-ar-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo- (9CI) (CA INDEX NAME)

D1-CO2H

CC 9-9 (Biochemical Methods)

IT Dyes

(fluorescent, intracellular fluorescent anions determination by cytoplasmic

dialysis of hepatocytes)

IT 475-31-0, Glycocholic acid 863-57-0D, reaction products with FITC 27072-45-3D, reaction products with sodium glycocholate 103991-76-0

RL: ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process)

(intracellular fluorescent anions determination by cytoplasmic dialysis of

hepatocytes)

L83 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

1993:444488 Document No. 119:44488 Correction of absorption spectra of a pH-sensitive dye for intracellular pH estimation in smooth

<WALKE 10/789566><Page 133>

muscle. Matsumoto, T.; Tomita, T. (Sch. Med., Nagoya Univ., Nagoya, 466,

Japan). Japanese Journal of Physiology, 43(1), 103-9 (English) 1993. CODEN: JJPHAM. ISSN: 0021-521X.

AB Methods of correction for intracellular pH (pHi) estimation from the absorbance

of the pH-sensitive dye, 4',5'-dimethyl-5-(and

-6-)carboxy-fluorescein (Me2CF), were described. In the guinea pig vena

cava, a reasonable estimation of pHi changes was obtained when the distortion

of the spectrum was corrected using the tissue absorbance at wavelengths longer

than 570 nm.

IT 103991-76-0

RL: ANST (Analytical study)

(in intracellular pH estimation in smooth muscle)

RN 103991-76-0 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-ar-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo- (9CI) (CA INDEX NAME)

 $D1-CO_2H$

CC 9-5 (Biochemical Methods)

Hq TI

(estimation of intracellular, in smooth muscle by spectrometry, pH-sensitive

dye in)

IT Muscle

(smooth, pH estimation in, by spectrometry pH-sensitive dye in)

IT 103991-76-0

RL: ANST (Analytical study)

<WALKE 10/789566><Page 134>

(in intracellular pH estimation in smooth muscle) 12408-02-5 IT RL: ANST (Analytical study) (pH, estimation of intracellular, in smooth muscle by spectrometry, pH-sensitive dye in) ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN 1989:487152 Document No. 111:87152 Photosensitized reduction of benzil by heteroatom-containing anthracene dyes. Shen, Tao; Zhao, Zhangong; Yu, Qun; Xu, Huijun (Inst. Photogr. Chem., Acad. Sin., Beijing, Peop. Rep. China). Journal of Photochemistry and Photobiology, A: Chemistry, 47(2), 203-12 (English) 1989. CODEN: JPPCEJ. 1010-6030. AB Benzil in MeOH was quant. reduced to benzoin by triethylamine in the presence of some heteroatom-containing anthracene dyes under visible irradiation The thermodn., kinetics, and various quantum yields were investigated. The transient intermediate of the reaction was detected by flash photolysis. The relation between the photosensitized reduction and the fading of the dyes was studied. The requirements for the dyes and the mechanism of these reactions were clarified. ΙT 122135-59-5 RL: RCT (Reactant); RACT (Reactant or reagent) (photoredn. of benzil sensitized by) 122135-59-5 HCAPLUS RN

Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

diiodo-2',7'-dimethyl-, disodium salt (9CI) (CA INDEX NAME)

CN

3', 6'-dihydroxy-4', 5'-

●2 Na

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

ST photoredn benzil sensitized anthracene dye

IT Reduction, photochemical

(of benzil, sensitized by heteroatom-containing anthracene dyes)

IT Energy level transition

(intersystem crossing, in photosensitized reduction of benzil by heteroatom-containing anthracene **dye**)

IT 119-53-9P, Benzoin

RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, in photosensitized reduction of, benzil by heteroatom-containing

croacom containing

anthracene dye)

IT 61-73-4, Methylene blue 65-61-2, Acridine orange 81-88-9,

Rhodamine B

.81-93-6, Phenosafranine 581-64-6, Thionine 1787-57-1, Capri blue 3474-67-7 11121-48-5, Rosebengal 16423-68-0 17372-87-1, Eosine 33239-19-9 122135-59-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (photoredn. of benzil sensitized by)

L83 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

1986:511334 Document No. 105:111334 Characteristics of fluoroprobes for measuring intracellular pH. Graber, Mark L.; DiLillo, Douglas C.; Friedman, Bradford L.; Pastoriza-Munoz, Enrique (Div. Nephrol.,

Veterans

Adm., Northport, NY, 11768, USA). Analytical Biochemistry, 156(1), 202-12

(English) 1986. CODEN: ANBCA2. ISSN: 0003-2697.

AB Four different fluoroprobes were evaluated to determine their capabilities and

<WALKE 10/789566><Page 136>

limitations in measuring intracellular pH by the fluorescent indicator technique with a fluorometer. In vitro, carboxyfluorescein, dimethylcarboxyfluorescein, bis(carboxyethyl)carboxyfluorescein, and 4-methylumbelliferone (4MU) all showed comparably intense fluorescence and

excellent pH sensitivity near their resp. pKa values. Major differences

were found between 4MU and the fluoresceins in terms of protein binding,

concentration effects, bleach rates, and the retention time within cells. Both

fluorescence and a fluorescence ratio at pH-sensitive/pH-insensitive excitation wavelengths increased with pH for all compds., and the ratio

completely corrected for large changes in the excitation light intensity. In

contrast, the ratio showed large artifactual changes as **dye** concentration increased because of self-quenching effects and spectral shifts.

Protein interactions likewise caused spectral shift and ratio aberrancies,

but Ca, Mg, and O had no effect on the fluorescence ratios. Apparently,

measurements of cell pH by fluorescence techniques are subject to artifacts induced by self-quenching and protein binding. Use of the fluorescence ratio technique does not necessarily correct for these artifacts, and in particular the ratio technique does not correct for changes in fluoroprobe concentration Because the major artifacts cause the

ratios for 4MU and for the fluoresceins to move in opposite directions, an

exptl. maneuver can cause a true change in pH if the fluorescence and ratios change in the same direction for these 2 classes of fluoroprobes.

IT 103991-76-0

RL: PROC (Process)

(in pH determination in cells, characterization of)

RN 103991-76-0 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-ar-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo- (9CI) (CA INDEX NAME)

 $D1-CO_2H$

CC 9-5 (Biochemical Methods)

IT 90-33-5 72088-94-9 85138-49-4 **103991-76-0**

RL: PROC (Process)

(in pH determination in cells, characterization of)

L83 ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
1986:65188 Document No. 104:65188 Intracellular calibration of a
pH-sensitive dye in isolated, perfused salamander proximal
tubules. Chaillet, J. Richard; Boron, Walter F. (Sch. Med., Yale
Univ.,

New Haven, CT, 06510, USA). Journal of General Physiology, 86(6), 765-94

(English) 1985. CODEN: JGPLAD. ISSN: 0022-1295.

AB The dyes 4',5'-dimethyl-5- (and -6-) carboxyfluorescein (Me2CF) were evaluated for determining the intracellular pH (pHi) of isolated, perfused

proximal tubules of salamander. The intracellular absorbance spectrum,

corrected for the intrinsic absorbance of the tubule, was obtained once per s.

The **dye** was incorporated into tubule cells by exposing them to the membrane-permeable precursor 4',5'-dimethyl-5- (and -6-) carboxyfluorescein diacetate. The introduction of the **dye** had no significant effect on either pHi or cell voltage transients. Compared

with **dye** contained in a cuvette, intracellular **dye** had a peak absorbance that was red-shifted by .apprx.5 nm and an apparent pK

that was increased by .apprx.0.3. These differences precluded an accurate

<WALKE 10/789566><Page 138>

calcn. of pHi by the comparison of intracellular spectra with in vitro calibration spectra. However, when Me2CF was calibrated intracellularly

by using the K-H exchanger nigericin to equalize external pH and pHi, the

dye-derived, steady state pHi was within .apprx.0.1 of the value obtained with pH-sensitive microelectrodes. Furthermore, when pHi was measured simultaneously with dye and microelectrodes during rapid pHi transients, the pHi time courses measured by the 2 methods were

very similar. Thus, the intracellular absorbance spectrum of Me2CF can be $\label{eq:canbara} % \begin{array}{c} \text{very similar.} \\ \text{very similar.} \end{array}$

used to measure steady-state pHi and rapid pHi transients reliably, provided the dye is calibrated intracellularly.

IT 100111-02-2 100111-03-3

RL: ANST (Analytical study)

(in intracellular pH determination in proximal tubule)

RN 100111-02-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

RN 100111-03-3 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-dihydroxy-4',5'-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 12

ST proximal tubule intracellular pH detn; dimethylcarboxyfluorescein pH detn;

spectrophotometry intracellular pH detn; fluorescein dimethylcarboxy pH

detn; salamander proximal tubule dye calibration

100111-02-2 100111-03-3 100111-04-4 100111-05-5

RL: ANST (Analytical study)

(in intracellular pH determination in proximal tubule)

L83 ANSWER 11 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN 1984:631930 Document No. 101:231930 Studies of the synthesis, properties,

and pharmacological activity of some new phthalein dyes and their mercury derivatives. Gupta, Anil K.; Srivastava, Anil K.; Srivastava, Nirupma; Lal, L. B. (Dep. Chem., K. G. K. Postgrad. Coll., Moradabad, India). Vijnana Parishad Anusandhan Patrika, 26(4), 319-25 (Hindi) 1983. CODEN: VPAPA9. ISSN: 0505-5806.

GI

ΙT

AB New phthalein-type dyes I [93376-43-3] and II (R = OH, Me; R1 = $_{\rm H}$, OH) were prepared by condensing 3-nitrophthalic acid [603-11-2] with

mono-, di- and trihydroxybenzenes in presence of concentrated H2SO4 as condensing agent. They were examined anal. and spectrophotometrically, and

some were mercurated. Na salts of these **dyes** and their Hg derivs. have bactericidal properties.

IT 93376-39-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study) (bactericidal activity of)

RN 93376-39-7 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one,

3',6'-dihydroxy-1',8'-

dimethyl-4-nitro-, sodium salt (9CI) (CA INDEX NAME)

●x Na

93376-30-8P IT

RN

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, mercuration and visible absorption of) 93376-30-8 HCAPLUS

Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, CN 3',6'-dihydroxy-1',8'-

dimethyl-4-nitro- (9CI) (CA INDEX NAME)

41-8 (Dyes, Organic Pigments, Fluorescent Brighteners, and CC Photographic

Sensitizers)

Section cross-reference(s): 63

STphthalein dye; nitrophthalein mercury bactericide

Bactericides, Disinfectants, and Antiseptics ΙT

(nitrophthalein dyes and their mercury derivs.)

ITDyes

<WALKE 10/789566><Page 142>

(nitrophthaleins and mercury derivs., preparation, bactericidal activity and

visible absorption of)

IT 93376-37-5 93376-38-6 **93376-39-7** 93376-40-0 93376-41-1 93376-42-2 93395-43-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)
 (bactericidal activity of)

IT 93376-29-5P **93376-30-8P** 93376-31-9P 93376-32-0P 93376-43-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, mercuration and visible absorption of)

L83 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
1971:45540 Document No. 74:45540 Determination of lipstick-colors.
Unterhalt, Bernard (Inst. Pharm. Chem. Lebensmittelchem., Univ. Marburg

Lahn, Marburg Lahn, Fed. Rep. Ger.). Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung, 144(2), 109-12 (German) 1970.

CODEN: ZLUFAR. ISSN: 0044-3026.

AB A chromatog. method is described using a 0.2 g. lipstick aliquot and petroleum ether and EtOH for estimation of the dyes (xanthene compds. and some pigments approved by German food and drug laws for the purpose).

Qual. thin-layer chromatog. with AcOEt-BuOH-concentrated NH4OH (20:-55:25) and

ProH-dilute NH4OH (90:10) as eluents on a 0.25 mm layer of silica gel ${\tt G}$ or ${\tt H}$

separated the **dyes**; preparative thin-layer chromatog. was performed with 20 + 40 cm plates of silica gel PF254 2 mm thick, with PrOH-NH4OH (9:1) as developer and MeOH as eluent. Quant. separation

purification of certain zones was most effectively accomplished by column

chromatog. on neutral or acid Al2O3, or neutral Al2O3 with PrOH-NH4OH for $\ensuremath{\text{NH4OH}}$

developing. Standard dyes were used in identifying the lipstick compds.

IT 32049-34-6

and

RL: ANT (Analyte); ANST (Analytical study) (determination of, in lipstick)

RN 32049-34-6 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-2'-(phenylmethyl)- (9CI) (CA INDEX NAME)

CC 62 (Essential Oils and Cosmetics)

ST lipstick colors detn; dyes lipsticks detn; colorants detn lipsticks; anal lipsticks

IT Cosmetics

(lipstick, anal. for xanthene dyes)

IT Dyes

(xanthene, determination in lipstick)

IT 548-26-5 568-63-8 596-03-2 632-68-8 2320-96-9 4618-23-9 6371-82-0 6441-77-6 24545-86-6 32021-46-8 **32049-34-6**RL: ANT (Analyte); ANST (Analytical study) (determination of, in lipstick)

L83 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

1964:425899 Document No. 61:25899 Original Reference No. 61:4518b-f Phthaleins and rhodamines derived from furan-2,3,4,5-tetra-carboxylic acid. Effect of replacing the benzene ring by a furan ring. Loiwal, S.

D.; Jain, N. C. (Birla Coll., Rajasthan). J. Indian Chem. Soc., 41(2),

150-4 (Unavailable) 1964.

GI For diagram(s), see printed CA Issue.

AB The effect of the furan nucleus on the ultraviolet absorption maximum of

various phthaleins and rhodamines was studied by preparing a number of the $% \left(1\right) =\left(1\right) +\left(1\right)$

dyes from furan-2,3,4,5-tetracarboxylic acid (I) and m-C6H4(OH)2 (II), 3,5-(HO)2C6H3Me (III), 1,3,5-C6H3(OH)3 (IV), 1,2,3-C6H3(OH)3 (V),

PhOH (VI), o-MeC6H4OH (VII), and m-Et2NC6H4OH (VIII). I was prepared as

follows: EtO2CCOCHNaCO2Et was coupled by means of Br in CHCl3 to [EtO2CCOCH(CO2Et)]2 which was cyclized with concentrated H2SO4 to the tetra-Et

ester (IX) of I. Hydrolysis of IX gave I, m. 247° (decompose) (Me2CO-C6H6). Compds. of general formulas X and XI were obtained by condensing I with II-VIII according to published procedures (Loiwal and

Jain, CA 59, 8902h). For example, heating 2.44 g. I with 5.0 g. II at $160\text{--}80^\circ$ for 3 hrs. in the presence of 3-4 drops concentrated H2SO4 gave X

(R1 = R2 = R4 = H, R3 = OH) (XII), m. 260° (decomposition). Other X and

XI were similarly prepared [formula, R1, R2, R3, R4, and m.p. (decomposition)

given]: X, Me, H, OH, H, >300°; X, OH, H, OH, H, >300°; X, H, H, OH, OH, >300°; X, H, H, NEt2, H, 206°; XI, OH, H, -, -, 155°; XI, OH, Me, -, -, 242°. X (R1 = H, R2 = R4 = Br R3 = OH), m. 152°, was prepared by brominating XII, and X (R1 = R2 = R4 = H, R3 =OAc), m. 215°, was obtained by acetylating XII with Ac2O in the presence of fused NaOAc. On comparing the absorption data, the replacement of the benzene ring with a furan ring had no appreciable effect. The slightly lower values obtained in some cases could be due to

the lower absorption maximum of furan. Colors of the dyes in EtOH and alkaline EtOH are given.

IT 100770-41-0, Fluorescein, 1',8'-dimethyl- (spectrum of)

RN 100770-41-0 HCAPLUS

CN Fluorescein, 1',8'-dimethyl- (7CI) (CA INDEX NAME)

CC 46 (Dyes)

IT Dves

(from 2,3,4,5-furantetracarboxylic acid and polyhydroxybenzene compds.)

IT 93044-50-9, 2,3,4,5-Furantetracarboxylic acid, 2,5-diethyl 3,4-di-Me ester

(in preparation of xanthene-type dyes)

IT 77-09-8, Phenolphthalein 2103-64-2, Gallein 2321-07-5, Fluorescein 2468-23-7, Fluoran, 1',3',6',8'-tetrahydroxy- 15086-94-9, Fluorescein,

2',4',5',7'-tetrabromo- 100770-41-0, Fluorescein,

1',8'-dimethyl-(spectrum of)

<WALKE 10/789566><Page 145>

L83 ANSWER 14 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

1964:31516 Document No. 60:31516 Original Reference No. 60:5668c-e **Dyes** derived from substituted phthalic acids. V.

3,6-Endoxohexahydrophthalic acid. Effect of completely saturating and

οf

introducing an oxygen bridge in the phthalic acid portion of phthalein dyes. Loiwal, S. D.; Jain, N. C. (Birla Coll., Rajasthan, India). J. Indian Chem. Soc., 40(9), 785-8 (Unavailable) 1963.

GI For diagram(s), see printed CA Issue.

AB cf. CA 60, 3129h. 3,6-Endoxohexahydrophthalic anhydride (I) when condensed with various phenols gave phthalein **dyes** similar spectrophotometrically to ones previously described. Thus, treatment of I

at temps. between 180 and 200° for 3-4 hrs. in the presence of a trace of H2SO4 and the appropriate phenol gave II which could be further

brominated or acetylated. Treatment of I at temps. between 110 and 120° for 14-20 hrs. in a similar manner gave III. The following II were prepared (R1, R2, R3, R4, and m.p. (decomposition) given): H, H, OH, H,

>300°; Me, H, OH, H, 225°; OH, H, OH, H, >300°; H, H, NEt2, H, >300°; H, Br, OH, Br, >300°; H, H, OAc, H,

220°. The following III were prepared (R1, R2, and m.p.

(decomposition)

given): OH, H, 225°; OH, Me, 210°.

IT 101358-43-4, 7-Oxabicyclo[2.2.1]heptane-2-carboxylic acid, 3-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone (preparation of)

RN 101358-43-4 HCAPLUS

CN 7-Oxabicyclo[2.2.1]heptane-2-carboxylic acid, 3-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ-lactone (7CI) (CA INDEX NAME)

```
CC
     46 (Dyes)
ΙT
     Dyes
        (phthalein, from 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid
and
        phenols)
     95814-21-4, 7-Oxabicyclo[2.2.1]heptane-2-carboxylic acid,
ΙT
     3-[hydroxybis(p-hydroxyphenyl)methyl]-, \gamma-lactone
                                                           96057-96-4,
     7-Oxabicyclo[2.2.1]heptane-2-carboxylic acid,
3-(3,6,9-trihydroxyxanthen-9-
     yl)-, γ-lactone
                        96058-01-4, 7-Oxabicyclo[2.2.1]heptane-2-
     carboxylic acid, 3-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, \gamma-lactone
     96058-24-1, 7-Oxabicyclo[2.2.1]heptane-2-carboxylic acid,
     3-(2,4,5,7-\text{tetrabromo}-3,6,9-\text{trihydroxyxanthen}-9-\text{yl})-, \gamma-\text{lactone}
     96173-05-6, 7-0xabicyclo[2.2.1]heptane-2-carboxylic acid,
     3-[hydroxybis(4-hydroxy-m-tolyl)methyl]-, \gamma-lactone
                                                             96708-26-8,
     7-Oxabicyclo[2.2.1]heptane-2-carboxylic acid,
3-(3,6,9-trihydroxyxanthen-9-
     yl)-, \gamma-lactone, diacetate 96931-53-2, 7-0xabicyclo[2.2.1]heptane-
     2-carboxylic acid, 3-[3,6-bis(diethylamino)-9-hydroxyxanthen-9-yl]-,
     \gamma-lactone 101358-43-4, 7-0xabicyclo[2.2.1]heptane-2-
     carboxylic acid, 3-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-,
     γ-lactone
        (preparation of)
     145-73-3, 7-0xabicyclo[2.2.1]heptane-2,3-dicarboxylic acid
ΙT
        (preparation of, and dyes from)
     ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
1964:17413
             Document No. 60:17413 Original Reference No. 60:3129h,3130a-b
     Dyes derived from substituted phthalic acids. IV.
     3,4-Dimethyl-5-ethyl-\Delta4-tetrahydrophthalic acid. Loiwal, S. D.;
     Jain, N. C. (Birla Coll., Rajasthan). J. Indian Chem. Soc., 40(8),
686-8
     (Unavailable) 1963.
GΙ
     For diagram(s), see printed CA Issue.
AB
     cf. CA 59, 8902h. Phthalein or rhodamine dyes were prepared by
     condensing 3,4-dimethyl-5-ethyl-\Delta4-tetrahydrophthalic anhydride (I)
     with phenols. Thus, treatment of I at 110-80° for 3-12 hrs. in the
     presence of a trace of H2SO4 and the appropriate phenol gave II or III
     which could be further brominated or acetylated. The following II
were
     prepared (R1, R2, R3, R4, m.p., color of crystals, color in EtOH and
in alkaline
     EtOH given): H, H, OH, H, 185°, reddish brown, orange-yellow, pink;
     Me, H, OH, H, 155°, brown, yellow, light pink; OH, H, OH, H,
     >300°, red, yellow, orange; H, H, NEt2, H, 165°, dark pink,
     pink, intense pink with 1 drop 5N HCl; H, Br, OH, Br, >300°, dark
     red, blood red, intense red; H, H, OAc, H, 120°, brown, yellow,
```

yellow. The following III were prepared (R and same data given): H,

<WALKE 10/789566><Page 147>

140°, light brown, yellow, light pink; Me, 165°, light brown, yellowish brown, dark pink.

IT 95622-65-4, 3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ-lactone 95622-74-5,
3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, γ-lactone 95958-60-4,
3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(2,4,5,7-tetrabromo-3,6,9-trihydroxyxanthen-9-yl)-, γ-lactone
102344-24-1, 3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ-lactone
(preparation of)

RN 95622-65-4 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 95622-74-5 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, γ-lactone (7CI) (CA INDEX NAME)

RN 95958-60-4 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(2,4,5,7-tetrabromo-3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 102344-24-1 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid,

4-ethyl-2,3-dimethyl-6-(3,6,9-trihydroxy-

1,8-dimethylxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

CC 46 (Dyes)

IT Dyes

(hydrogenated fluoran derivs.)

IT 95622-08-5, 3-Cyclohexene-1-carboxylic acid, 4-ethyl-6-[hydroxybis(p-hydroxyphenyl)methyl]-2,3-dimethyl-, γ-lactone 95622-65-4,
3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ-lactone 95622-74-5,
3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, γ-lactone 95958-60-4,
3-Cyclohexene-1-carboxylic acid, 4-ethyl-2,3-dimethyl-6-(2,4,5,7-

<WALKE 10/789566><Page 149>

tetrabromo-3, 6, 9-trihydroxyxanthen-9-yl)-, γ -lactone 96215-28-0, 3-Cyclohexene-1-carboxylic acid, 4-ethyl-2, 3-dimethyl-6-(3, 6, 9trihydroxyxanthen-9-yl)-, γ -lactone, diacetate 96765-30-9, 3-Cyclohexene-1-carboxylic acid, 4-ethyl-6-[hydroxybis(4-hydroxy-mtolyl)methyl]-2,3-dimethyl-, γ -lactone 102344-24-1, 3-Cyclohexene-1-carboxylic acid, 4-ethyl-2, 3-dimethyl-6-(3, 6, 9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone (preparation of) ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L83 1963:448869 Document No. 59:48869 Original Reference No. 59:8902h,8903a-d Dyes derived from substituted phthalic acids. III. cis- $\Delta 4$ -Tetrahydrophthalic acid. Effect of decreasing unsaturation in the phthalic acid portion of phthalein dyes. Loiwal, S. D.; Jain, N. C. (Birla Coll., Pilani, India). J. Indian Chem. Soc., 39, 745 - 8(Unavailable) 1962. For diagram(s), see printed CA Issue. GΙ AB cf. CA 58, 601b, 5813q. cis- $\Delta 4$ -Tetrahydrophthalic anhydride (I) was prepared and condensed with several phenols and with m-Et2NC6H4OH (II) to the corresponding phthaleins and rhodamine-type compds., resp., which were studied anal. and spectrophotometrically. The phthalein from m-C6H4 (OH) 2 (III) was also brominated and acetylated. Decreasing unsatn. in the phthalic acid portion of the dyes causes only slight variations in the absorption maximum as compared to the corresponding phthaleins for the condensation products from o-MeC6H4OH and 3,5-(HO)2C6H3Me with I but not for the dyes from 1,3,5-C6H3(OH)3 and II with I which show absorption maximum in the same region as the corresponding phthaleins. 1,3-Butadiene passed into 500 cc. dry C6H6 and 196 g. maleic anhydride yielded I, m. 103-4° (ligroine), which was hydrolyzed to the corresponding acid, m. 163-4°. I (2.5 g.) and 4.0 g. III heated 3 hrs. at 160-80° in the presence of 4-5 drops concentrated H2SO4 gave IV (R1, R2, R4 = H; R3 = OH) (V), reddish brown, m. 245° (decomposition), orange in EtOH, pink with green fluorescence in alkaline EtOH. Similarly were prepared the following IV (R1, R2, R3, R4, m.p., reaction temperature, reaction time in hrs., color of crystals, color in EtOH, and color in alkaline EtOH given): Me, H, OH, H, 220° (decomposition), 140-60°, 4,

brown-red, yellow, light pink with green fluorescence; OH, H, OH, H, 280°, 180-200°, 3, red, orange, orange-red; H, H, NEt2, H,

118°, 100-5°, 3, pink, pink, -(pink in HCl-EtOH). I (2.5

g.) and 6 g. o-MeC6H4OH heated 14 hrs. at 110-15° with 8 drops concentrated H2SO4 gave VI, whitish brown, m. 165° (decomposition), yellow in

EtOH, purple-pink in alkaline EtOH. V brominated gave the pink-red tetrabromo

derivative, m. 200 $^{\circ}$ (decomposition), blood-red in EtOH, deep pink in alkaline

EtOH. V with NaOAc-Ac2O yielded the yellow-brown diacetate, m. 190°, yellow in EtOH and alkaline EtOH. The ultraviolet absorption maximum of the IV and V in neutral and alkaline alc. medium are tabulated and

compared with those of the corresponding phthaleins.

IT 101358-41-2, 3-Cyclohexene-1-carboxylic acid, 6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone (preparation of)

RN 101358-41-2 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid,

6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

CC 46 (Dyes)

IT Dves

(from phthalic acid derivs.)

IT Unsaturation

(in phthalein dyes, effect of decrease in)

IT 88-99-3, Phthalic acid (derivs., dyes from)

IT 85-43-8, 4-Cyclohexene-1,2-dicarboxylic anhydride 94465-41-5,
3-Cyclohexene-1-carboxylic acid, 6-(3,6,9-trihydroxyxanthen-9-yl)-,
γ-lactone 94544-86-2, 3-Cyclohexene-1-carboxylic acid,
6-(2,4,5,7-tetrabromo-3,6,9-trihydroxyxanthen-9-yl)-, γ-lactone
95957-69-0, 3-Cyclohexene-1-carboxylic acid,

6-(3,6,9-trihydroxyxanthen-9-

```
yl)-, γ-lactone, diacetate
                                    96057-99-7, 3-Cyclohexene-1-carboxylic
     acid, 6-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, \gamma-lactone
     96172-94-0, 3-Cyclohexene-1-carboxylic acid,
6-[hydroxybis(4-hydroxy-m-
     tolyl)methyl]-, \gamma-lactone 96274-84-9, 3-Cyclohexene-1-carboxylic
     acid, 6-[3,6-bis(diethylamino)-9-hydroxyxanthen-9-yl]-, \gamma-lactone
     101358-34-3, 2,7-Naphthalenedisulfonic acid, 3-hydroxy-, compound
with C.I.
     Basic Orange 2 (1:1) 101358-41-2, 3-Cyclohexene-1-carboxylic
     acid, 6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, \gamma-lactone
     104157-77-9, 1-Anthracenesulfonic acid, 9,10-dihydro-9,10-dioxo-,
compound
     with C.I. Basic Orange 2 105666-86-2, 2,7-Naphthalenedisulfonic
acid,
     3-hydroxy-, compound with C.I. Basic Orange 2 (1:2)
                                                               105948-76-3,
     1,8-Anthracenedisulfonic acid, 9,10-dihydro-9,10-dioxo-, compound
with C.I.
     Basic Orange 2
        (preparation of)
     88-98-2, 4-Cyclohexene-1,2-dicarboxylic acid
ΙT
        (preparation of, for dyes)
    ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
L83
            Document No. 58:33818 Original Reference No. 58:5814b-d
     Dyes derived from substituted phthalic acids II.
     3, 4, 5, 6-Tetraphenyl and 3, 4, 5, 6-tetraphenyl-\Delta.5-dihydrophthalic
     acids. Effect of introducing phenyl groups in the phthalic and partly
     saturated phthalic acids. Loiwal, S. D.; Tewari, J. D. (Univ.
Allahabad,
     India).
               J. Indian Chem. Soc., 39, 646-50 (Unavailable) 1962.
AB
     Other phthaleins were prepared similarly by using 3,4,5,6-
     tetraphenylphthalic anhydride and 3,4,5,6-tetraphenyl-\Delta3.5-
     dihydrophthalic anhydride. The following 3,4,5,6-tetraphenyl derivs.
of I
     were prepared (R, R1, R2, R3, R4, and m.p. given): --, H, H, OH, H,
     285°; Δ3.5-dihydro, H, H, OH, H, 255°; --, Me, H, OH,
     H, 220°; Δ3.5-dihydro, Me, H, OH, H, 245°; --, OH, H,
     OH, H, 270°; Δ3.5-dihydro, OH, H, OH, H, >300°; --, H,
     H, OH, OH, >300^\circ; \Delta 3.5-dihydro, H, H, OH, OH, 220°;
     --, H, H, H, OH, >300^{\circ}; \Delta 3.5-dihydro, H, H, H, OH,
     285°; --, H, OH, H, H, 235°; Δ3.5-dihydro, H, OH, H,
     H, 255°; --, H, Br, OH, Br, 255°; Δ3.5-dihydro, H, Br,
     OH, Br, 225^{\circ}; --, H, H, OAc, H, 272^{\circ}; \Delta 3.5-dihydro, H, H, OAc, H, 283^{\circ}. The following II were prepared (R, R1, and m.p.
     given): --, H, 205°; Δ3.5-dihydro, H, 130°; --, Me,
     280°; Δ3.5-dihydro, Me, 265°. A comparative study of
     the absorption maximum of the dyes showed that the introduction of
     Ph groups in the phthalic and dihydrophthalic portions of the dye
```

<WALKE 10/789566><Page 152>

mols. did not affect the light absorption appreciably. Introduction of Ph

groups in the phthalic acid portion increased the color intensity.

106298-79-7, Fluorescein, 1',8'-dimethyl-4,5,6,7-tetraphenyl-107542-03-0, 2,4-Cyclohexadiene-1-carboxylic acid,

10/542-03-0, 2,4-Cyclonexadiene-i-carboxylic acid,

2,3,4,5-tetraphenyl-6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone

(preparation and spectrum of)

RN 106298-79-7 HCAPLUS

ΙT

CN Fluorescein, 1',8'-dimethyl-4,5,6,7-tetraphenyl- (7CI) (CA INDEX NAME)

RN 107542-03-0 HCAPLUS

CN 2,4-Cyclohexadiene-1-carboxylic acid, 2,3,4,5-tetraphenyl-6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

CC 46 (Dyes)

IT Dyes

(from phthalic acid derivs.)

```
Spectra, visible and ultraviolet
ΙT
        (of dyes, from substituted phthalic acids)
     88-99-3, Phthalic acid
ΙT
        (derivs., dyes from)
ΙT
     28672-71-1, 2,4-Cyclohexadiene-1-carboxylic acid, <math>6-(4,5,9-1)
     trihydroxyxanthen-9-yl)-, \gamma-lactone
                                             28672-72-2,
     2,4-Cyclohexadiene-1-carboxylic acid,
6-(3,4,5,6,9-pentahydroxyxanthen-9-
                        28745-11-1, 2,4-Cyclohexadiene-1-carboxylic acid,
     yl)-, γ-lactone
     6-(2,7,9-trihydroxyxanthen-9-yl)-, \gamma-lactone
                                                     80218-28-6,
     Phenolphthalein, 4,5,6,7-tetraphenyl-
                                               88856-55-7,
1,5-Cyclohexadiene-1-
     carboxylic acid, 6-(3,6,9-trihydroxyxanthen-9-yl)-, \gamma-lactone,
                 88856-56-8, 2,4-Cyclohexadiene-1-carboxylic acid,
     6-(3,6,9-trihydroxyxanthen-9-yl)-, \gamma-lactone, diacetate
     94546-86-8, 1,5-Cyclohexadiene-1-carboxylic acid,
6-(2,4,5,7-tetrabromo-
     3,6,9-trihydroxyxanthen-9-yl)-, \gamma-lactone
                                                   94688-76-3,
     1,5-Cyclohexadiene-1-carboxylic acid,
6-(2,7,9-trihydroxyxanthen-9-yl)-,
                 94688-78-5, 1,5-Cyclohexadiene-1-carboxylic acid,
     γ-lactone
     6-(4,5,9-trihydroxyxanthen-9-yl)-, \gamma-lactone
                                                      95424-74-1,
     2,4-Cyclohexadiene-1-carboxylic acid, 6-(2,4,5,7-tetrabromo-3,6,9-
     trihydroxyxanthen-9-yl)-, \gamma-lactone
                                            96057-85-1,
     1,5-Cyclohexadiene-1-carboxylic acid, 6-[hydroxybis(p-
     hydroxyphenyl)methyl]-, \gamma-lactone 96057-86-2, 2,4-Cyclohexadiene-1-
     carboxylic acid, 6-[hydroxybis(p-hydroxyphenyl)methyl]-, \gamma-lactone
     96457-25-9, 1,5-Cyclohexadiene-1-carboxylic acid,
6-[hydroxybis(4-hydroxy-
     m-tolyl) methyl]-, \gamma-lactone 96972-19-9, 2,4-Cyclohexadiene-1-
     carboxylic acid,
2,3,4,5-tetraphenyl-6-(2,7,9-trihydroxyxanthen-9-yl)-,
                 96972-20-2, 2,4-Cyclohexadiene-1-carboxylic acid,
     γ-lactone
     2,3,4,5-tetraphenyl-6-(4,5,9-trihydroxyxanthen-9-yl)-, \gamma-lactone
     96972-22-4, 2,4-Cyclohexadiene-1-carboxylic acid, 6-[hydroxybis(p-
     hydroxyphenyl) methyl] -2, 3, 4, 5-tetraphenyl-, \gamma-lactone
                                                                97086-05-0,
     2,4-Cyclohexadiene-1-carboxylic acid, 2,3,4,5-tetraphenyl-6-(2,4,5,7-
     tetrabromo-3, 6, 9-trihydroxyxanthen-9-yl)-, \gamma-lactone 97118-22-4,
     2,4-Cyclohexadiene-1-carboxylic acid, 2,3,4,5-tetraphenyl-6-(3,6,9-
     trihydroxyxanthen-9-yl)-, \gamma-lactone, diacetate 97922-80-0,
     2,4-Cyclohexadiene-1-carboxylic acid,
6-(1,3,6,8,9-pentahydroxyxanthen-9-
     yl)-2,3,4,5-tetraphenyl-, \gamma-lactone
                                             97922-81-1,
     2,4-Cyclohexadiene-1-carboxylic acid,
6-(3,4,5,6,9-pentahydroxyxanthen-9-
     yl)-2,3,4,5-tetraphenyl-, \gamma-lactone
                                            98016-47-8,
     2,4-Cyclohexadiene-1-carboxylic acid, 6-[hydroxybis(4-hydroxy-m-
     tolyl)methyl]-2,3,4,5-tetraphenyl-, \gamma-lactone 98945-84-7,
```

```
2,4-Cyclohexadiene-1-carboxylic acid, 2,3,4,5-tetraphenyl-6-(3,6,9-
     trihydroxyxanthen-9-yl)-, \gamma-lactone 106298-79-7,
     Fluorescein, 1',8'-dimethyl-4,5,6,7-tetraphenyl- 106545-53-3,
Fluoran,
     3', 4', 5', 6'-tetrahydroxy-4, 5, 6, 7-tetraphenyl- 106545-54-4, Fluoran,
     1',3',6',8'-tetrahydroxy-4,5,6,7-tetraphenyl- 106545-55-5,
Fluorescein,
     4,5,6,7-tetraphenyl- 106545-56-6, Fluoran, 4',5'-dihydroxy-4,5,6,7-
     tetraphenyl- 106545-57-7, Fluoran,
2',7'-dihydroxy-4,5,6,7-tetraphenyl-
     106630-26-6, Fluorescein, 2',4',5',7'-tetrabromo-4,5,6,7-tetraphenyl-
     106767-50-4, Fluorescein, 4,5,6,7-tetraphenyl-, diacetate
107542-02-9,
     Phenolphthalein, 3',3''-dimethyl-4,5,6,7-tetraphenyl- 107542-03-0
       2,4-Cyclohexadiene-1-carboxylic acid, 2,3,4,5-tetraphenyl-6-(3,6,9-
     trihydroxy-1,8-dimethylxanthen-9-yl)-, \gamma-lactone
         (preparation and spectrum of)
L83
     ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
1963:33817
            Document No. 58:33817 Original Reference No.
58:5813q-h,5814a-d
     Dyes derived from substituted phthalic acids I.
     82.6-Dihydrophthalic and trans-83.5-dihydrophthalic acids.
     Effect of decreasing unsaturation in the phthalic acid portion of
     phthalein dyes. Loiwal, S. D.; Tewari, J. D. (Univ. Allahabad,
              J. Indian Chem. Soc., 39, 641-5 (Unavailable) 1962.
     India).
     For diagram(s), see printed CA Issue.
GΙ
     cf. CA 58, 601b. Various phthaleins I and II were prepared by
AΒ
condensing
     either \delta 2.6-di-hydrophthalic acid (III) or trans-\delta 3.5-
     dihydrophthalic acid (IV) with different phenols. The I and II were
     compared with phthaleins from o-C6H4(CO2H)2; decreasing unsatn. in
     the phthalic acid portion of phthaleins did not change the \lambda X max.
     Phthaleins from IV had more color intensity than plithaleins from
either
     o-C6H4(CO2H)2 or III. Thus, treatment of III or IV at temps.
     between 160-200° for 3 hrs. in the presence of a trace of H2SO4 and
     the appropriate phenol gave I which could be further brominated or
     acetylated. The following dihydro-I were prepared [R (denotes
     dihydrophthalein type), R1, R2, R3, R4, and m.p. given]: \Delta2.6, H, H,
     OH, H, 222^{\circ}; trans-\Delta 3.5, H, H, OH, H, 285^{\circ};
     \Delta 2.6, Me, H, OH, H, 205^{\circ}; trans-\Delta 3.5, Me, H, OH, H,
     220°; \Delta2.6, OH, H, OH, H, >300°; trans-\Delta3.5, OH,
     H, OH, H, >300^{\circ}; \Delta 2.6, H, H, OH, OH, >300^{\circ};
     trans-\Delta 3.5, H, H, OH, OH, >300°; \Delta 2.6, H, H, H, OH,
     >300^{\circ}; trans-\Delta 3.5, H, H, H, OH, >300^{\circ}; \Delta 2.6, H,
     OH, H, H, 270^{\circ} (decomposition); trans-\Delta 3.5, H, OH, H, H,
     >300^{\circ}; \Delta 2.6, H, Br, OH, Br, 200^{\circ}; trans-\Delta 3.5, H,
```

<WALKE 10/789566><Page 155>

Br, OH, Br, 220°; Δ2.6, H, H, OAc, H, 155°; trans- Δ 3.5, H, H, OAc, H, 235°. Treating III or IV with excess phenol and heating 10-14 hrs. at 105-20° gave II. following dihydro II were prepared (R, R1, and m.p. given): $\Delta 2.6$, H, 244°; trans- Δ 3.6, H, 170°; δ 2.6, Me, 150°; trans- Δ 3.5, Me, 148°. Colors of the various compds. and their solns. are given ΙT 100734-04-1, 1,5-Cyclohexadiene-1-carboxylic acid, 6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone 100802-83-3, 2,4-Cyclohexadiene-1-carboxylic acid, 6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone (preparation and spectrum of) RN 100734-04-1 HCAPLUS 1,5-Cyclohexadiene-1-carboxylic acid, 6-(3,6,9-trihydroxy-1,8-CN dimethylxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 100802-83-3 HCAPLUS
CN 2,4-Cyclohexadiene-1-carboxylic acid, 6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ-lactone (7CI) (CA INDEX NAME)

CC 46 (Dyes)
IT Dyes

Dyes

(from phthalic acid derivs.)

```
ΙT
     Spectra, visible and ultraviolet
     Spectra, visible and ultraviolet
        (of dyes, from substituted phthalic acids)
ΙT
     88-99-3, Phthalic acid
        (derivs., dves from)
ΙT
     4435-09-0, 2,4-Cyclohexadiene-1-carboxylic acid, 6-(3,6,9-
     trihydroxyxanthen-9-yl)-, \gamma-lactone
                                             28672-71-1.
     2,4-Cyclohexadiene-1-carboxylic acid,
6-(4,5,9-\text{trihydroxyxanthen}-9-\text{yl})-,
                 28672-72-2, 2,4-Cyclohexadiene-1-carboxylic acid,
     γ-lactone
     6-(3,4,5,6,9-pentahydroxyxanthen-9-y1)-, \gamma-lactone 28745-11-1,
     2,4-Cyclohexadiene-1-carboxylic acid,
6-(2,7,9-trihydroxyxanthen-9-yl)-,
                 88856-55-7, 1,5-Cyclohexadiene-1-carboxylic acid,
     γ-lactone
     6-(3,6,9-trihydroxyxanthen-9-yl)-, \gamma-lactone, diacetate
     88856-56-8, 2,4-Cyclohexadiene-1-carboxylic acid, 6-(3,6,9-
     trihydroxyxanthen-9-yl)-, \gamma-lactone, diacetate
                                                        94546-86-8,
     1,5-Cyclohexadiene-1-carboxylic acid, 6-(2,4,5,7-tetrabromo-3,6,9-
     trihydroxyxanthen-9-yl)-, γ-lactone
                                             94688-76-3,
     1,5-Cyclohexadiene-1-carboxylic acid,
6-(2,7,9-trihydroxyxanthen-9-yl)-,
     γ-lactone
                 94688-77-4, 1,5-Cyclohexadiene-1-carboxylic acid,
     6-(3,6,9-trihydroxyxanthen-9-yl)-, \gamma-lactone
                                                      94688-78-5,
     1,5-Cyclohexadiene-1-carboxylic acid,
6-(4,5,9-trihydroxyxanthen-9-yl)-,
                 94688-93-4, 1,5-Cyclohexadiene-1-carboxylic acid,
     γ-lactone
     6-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, \gamma-lactone 94688-94-5,
     1,5-Cyclohexadiene-1-carboxylic acid,
6-(3, 4, 5, 6, 9-pentahydroxyxanthen-9-
                        95424-74-1, 2,4-Cyclohexadiene-1-carboxylic acid,
     yl)-, γ-lactone
     6-(2,4,5,7-\text{tetrabromo}-3,6,9-\text{trihydroxyxanthen}-9-\text{yl})-, \gamma-\text{lactone}
     95743-08-1, 2,4-Cyclohexadiene-1-carboxylic acid, 6-(1,3,6,8,9-
     pentahydroxyxanthen-9-yl)-, \gamma-lactone 96057-85-1,
     1,5-Cyclohexadiene-1-carboxylic acid, 6-[hydroxybis(p-
     hydroxyphenyl)methyl]-, \gamma-lactone 96057-86-2, 2,4-Cyclohexadiene-1-
     carboxvlic acid, 6-[hydroxybis(p-hydroxyphenyl)methyl]-, \gamma-lactone
     96457-25-9, 1,5-Cyclohexadiene-1-carboxylic acid,
6-[hydroxybis(4-hydroxy-
     m-tolyl) methyl]-, \gamma-lactone 100734-04-1,
     1,5-Cyclohexadiene-1-carboxylic acid, 6-(3,6,9-trihydroxy-1,8-
     dimethylxanthen-9-yl)-, \gamma-lactone 100802-83-3,
     2,4-Cyclohexadiene-1-carboxylic acid, 6-(3,6,9-trihydroxy-1,8-
     dimethylxanthen-9-yl)-, \gamma-lactone
        (preparation and spectrum of)
```

ANSWER 19 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Dyes derived from 3-methyl- $\Delta 4$ -tetrahydrophthalic acids. II.

Document No. 58:3590 Original Reference No. 58:601b-h,602a-b

L83

1963:3590

Effect of introducing a methyl group at different positions (3 or 4) and

also of decreasing unsaturation in the phthalic acid portion of phthalein

dyes. Loiwal, S. D.; Jain, N. C. (Birla Coll., Pilani). Journal
 of the Indian Chemical Society, 39, 385-90 (Unavailable) 1962.
CODEN:

JICSAH. ISSN: 0019-4522.

of

GI For diagram(s), see printed CA Issue.

AB cf. CA 57, 6071c. 3-Methyl- $\Delta 4$ -tetrahydrophthalic anhydride (I) and its 4-Me isomer (II) were condensed with a series of phenols and with m-Et2NC6H4OH (IIa) to yield phthalein and rhodamine derivs. which were studied analytically and spectrophotometrically and compared with similar

compds. obtained fromo-C6H4(CO2H)2. The resorcinol derivs. were also brominated and acetylated. The effect of introducing a Me group at

the 3- or 4-position and also of decreasing the unsatn. in the ${\tt phthalic}$

acid portion of the phthaleins is discussed. I (1.66 g.) and 2.2 g. m-C6H4(OH)2 treated at 160° with 3-4 drops concentrated H2SO4, heated 3

hrs. at 180° , cooled, and extracted with dilute aqueous NaOH, and the filtered extract acidified with dilute HCl gave III (R1, R2, R4 = H, R3 = OH)

(IV), brick-red crystals, m. 220° (decomposition) (EtOH), grown-red in EtOH, changing to reddish with green fluorescence with alkali. II (1.66

g.) and 2.2 g. m-C6H4(OH)2 gave similarly the 4-Me isomer (V) of IV, reddish brown, m. 240° (decomposition), reddish brown in EtOH, changing

to reddish with green fluorescence with alkali. I (1.66 g.) and 2.48 g.

orcinol (VI) heated 4 hrs. at $140-50^{\circ}$ with 3-4 drops concentrated H2SO4

gave III (R1 = Me, R2, R4 = H, R3 = OH) (VII), dark red, m. $160-5^{\circ}$ (decomposition), yellow in EtOH changing to orange-red with green fluorescence

with alkali. II (1.66 g.) and 2.48 g. VI heated 5 hrs. at 115-20° with 3-4 drops concentrated H2SO4 yielded the 4-Me isomer of VII, dark red, m.

135° (decomposition), yellow in EtOH, changing to orange-green with alkali. I (1.66 g.) and 2.52 g. phloroglucinol (VIII) gave during 4 hrs.

at 180-200° III (R1, R3 = OH, R2, R4 = H) (IX), orange-red, m. >290° (decomposition), yellow in EtOH, changing to orange-red with alkali. II (1.66 g.) and 2.52 g. VII gave similarly the 4-Me isomer

- IX, orange-red, m. 260° (decomposition), yellow in EtOH, changing to orange-red with alkali. I (1.66 g.) and 2.82 g. IIa heated about 5 hrs.
- at 110-15° with concentrated H2SO4, powdered, and extracted with dilute HCl,
- and the extract acidified with dilute aqueous NaOH precipitated III (R1, R2, R4 = H, R3 = $\frac{1}{2}$
- NEt2) (X), dark pink, m. 120° (decomposition) (EtOH), deep pink in EtOH,
- intensified with HCl. II (1.66 g.) and 2.82 g. IIa gave similarly the 4-Me isomer of X, red, m. 147 $^{\circ}$ (decomposition), pink in EtOH, intensified with HCl. Bromination of IV gave III (R1 = H, R2, R4 = Br, R3
- = OH) (XI), dark red, m. $> 300^{\circ}$ (decomposition), brick red in EtOH, changing to deep pink with alkali. Similarly prepared was the 4-Me isomer
- of XI, dark red, m. $> 300^{\circ}$ (decomposition), brick-red in EtOH, changing
- to deep pink with alkali. IV refluxed with Ac2O and NaOAc yielded the diacetate (XII) of IV, brown, m. 145° (decomposition) (EtOH). The 4-Me
- isomer of XII, yellow-brown, m. 155° (decomposition), was prepared similarly. I (1.66 g.) and 3 g. PhOH heated 14 hrs. at 110-15° with 8 drops concentrated H2SO4, dissolved in 50 cc. H2O, blown with steam, and
- filtered, the residue extracted with aqueous NaOH, and the extract acidified with
- dilute HCl yielded XIII (R = OH, R' = H) (XIV), pinkish white powder,
- 125° (decomposition), yellowish brown in EtOH, changing to pink with alkali. II (1.66 g.) and 3 g. PhOH gave similarly the 4-Me isomer of XIV,
- brownish white powder, m. 147 $^{\circ}$ (decomposition), yellowish brown in EtOH,
- changing to pink with alkali. I (1.66 g.) and 3 g.o-MeC6H4OH gave in the same manner XIII (R = OH, R' = Me) (XV), pinkish white powder, m.
- 150° (decomposition), reddish brown in EtOH changing to purple pink with
- alkali. II (1.66 g.) and 3.5 g.o-MeC6H4OH gave the 4-Me isomer of XV, pinkish white powder, brown in EtOH, changing to purple pink with alkali. A comparative study of the absorption maximum of the various phthaleins and rhodamines showed that introduction of 3- and 4-Me groups
 - and decreasing the unsatn. in the phthalic acid portion have no appreciable effect on the light absorption, except in the $\tt dyes$ from o-MeC6H4OH and from VI and to some extent in the derivs. from m-C6H4(OH)2.

ΙT 94867-05-7, 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(3,6,9trihydroxyxanthen-9-yl)-, γ -lactone 94867-06-8, 3-Cyclohexene-1-carboxylic acid, 3-methyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone 94867-16-0, 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, γ -lactone 95947-27-6, 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(2,4,5,7tetrabromo-3, 6, 9-trihydroxyxanthen-9-yl)-, γ -lactone 95947-28-7, 3-Cyclohexene-1-carboxylic acid, 3-methyl-6-(2,4,5,7tetrabromo-3, 6, 9-trihydroxyxanthen-9-yl)-, γ -lactone 104878-73-1, 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(3,6,9trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone 107136-85-6 , 3-Cyclohexene-1-carboxylic acid, 3-methyl-6-(3,6,9-trihydroxy-1,8dimethylxanthen-9-yl)-, γ -lactone (preparation of) RN 94867-05-7 HCAPLUS CN 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 94867-06-8 HCAPLUS CN 3-Cyclohexene-1-carboxylic acid, 3-methyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 94867-16-0 HCAPLUS
CN 3-Cyclohexene-1-carboxylic acid,
2-methyl-6-(1,3,6,8,9-pentahydroxyxanthen9-yl)-, γ-lactone (7CI) (CA INDEX NAME)

RN 95947-27-6 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(2,4,5,7-tetrabromo-3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 95947-28-7 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid, 3-methyl-6-(2,4,5,7-tetrabromo-3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 104878-73-1 HCAPLUS

. CN 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 107136-85-6 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid, 3-methyl-6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

CC 46 (Dyes)

IT Dyes

ΙT

(phthalein, from 3-methyl- $\Delta 4$ -tetrahydrophthalic acid) 15941-50-1, 4-Cyclohexene-1,2-dicarboxylic acid, 3-methyl-

(dyes from)

IT 94867-05-7, 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone 94867-06-8,

3-Cyclohexene-1-carboxylic acid,

3-methyl-6-(3,6,9-trihydroxyxanthen-9-yl)-

, γ -lactone 94867-16-0, 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, γ -lactone 95817-45-1, 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone, diacetate 95938-70-8,

3-Cyclohexene-1-carboxylic acid,

6-[hydroxybis(p-hydroxyphenyl)methyl]-2-

methyl-, γ -lactone 95938-71-9, 3-Cyclohexene-1-carboxylic acid, 6-[hydroxybis(p-hydroxyphenyl)methyl]-3-methyl-, γ -lactone 95947-27-6, 3-Cyclohexene-1-carboxylic acid, 2-methyl-6-(2,4,5,7-

```
tetrabromo-3, 6, 9-trihydroxyxanthen-9-yl)-, \gamma-lactone
     95947-28-7, 3-Cyclohexene-1-carboxylic acid, 3-methyl-6-(2,4,5,7-
     tetrabromo-3, 6, 9-trihydroxyxanthen-9-yl)-, \gamma-lactone 96267-38-8,
     3-Cyclohexene-1-carboxylic acid,
6-[hydroxybis(4-hydroxy-m-tolyl)methyl]-2-
     methyl-, γ-lactone
                          96269-24-8, 3-Cyclohexene-1-carboxylic acid,
     6-[3,6-bis(diethylamino)-9-hydroxyxanthen-9-yl]-2-methyl-, \gamma-lactone
     97257-17-5, 3-Cyclohexene-1-carboxylic acid, 3-methyl-6-(3,6,9-
     trihydroxyxanthen-9-yl)-, \gamma-lactone, diacetate
     3-Cyclohexene-1-carboxylic acid,
6-[hydroxybis(4-hydroxy-m-tolyl)methyl]-3-
     methyl-, \gamma-lactone 104878-73-1, 3-Cyclohexene-1-carboxylic
     acid, 2-methyl-6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-,
     \gamma-lactone 107136-85-6, 3-Cyclohexene-1-carboxylic acid,
     3-methyl-6-(3,6,9-trihydroxy-1,8-dimethylxanthen-9-yl)-, \gamma-lactone
     108042-44-0, 3-Cyclohexene-1-carboxylic acid,
6-[3,6-bis(diethylamino)-9-
     hydroxyxanthen-9-yl]-3-methyl-, \gamma-lactone
        (preparation of)
     ANSWER 20 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
L83
              Document No. 57:30119 Original Reference No. 57:6071c-h
     Dyes derived from 4,5-dimethyl-\Delta 4-tetrahydrophthalic acid.
     I. Effect of introducing methyl groups and also of decreasing
unsaturation
     in the phthalic acid portion of phthalein dyes. Loiwal, S. D.;
     Jain, N. C. (Birla Coll., Pilani). J. Indian Chem. Soc., 39, 251-4
     (Unavailable) 1962.
GΙ
     For diagram(s), see printed CA Issue.
     4,5-Dimethyl-\Delta 4-tetrahydrophthalic anhydride (I) [m. 78-9°
AΒ
     (petr. ether)] (Farmer and Warren, CA 23, 3674) was condensed with a
number
     of phenols and with m-Et2NC6H4OH (II). The resulting dyes (III
     and IV) were compared spectrophotometrically with similar dyes
     obtained from phthalic acid. I (2 g.) and 2.5 g. resorcinol heated to
     160°, the mixture treated with 3-4 drops concentrated H2SO4, heated 3
hrs.
     at 180°, cooled, extracted with dilute NaOH, and the filtered extract
     treated portionwise with dilute HCl gave III (R = R' = R'' = H, R''
= OH)
     (V), m. 210° (decomposition) (repptn. from alkaline solution, then
EtOH).
     Similarly dyes were prepared (phenol, R, R', R'', R''' of III, and m.p. given): orcinol, Me, H, OH, H, 200^{\circ} (decomposition) (purified as
     above); phloroglucinol, OH, H, OH, H, 245° (decomposition);
pyrogallol,
     H, H, OH, OH, 230^{\circ} (decomposition); and II, H, H, NEt2, H, >300^{\circ}.
     V brominated by the method of Baeyer (Ann. 183, 3(1876)) gave III (R
= H,
```

<WALKE 10/789566><Page 164>

R' = R''' = Br, R'' = OH), m. >300°. Acetylation of V with Ac20-fused NaOAc gave III (R = R' = R''' = H, R'' = Ac), m. 150° (decomposition) (EtOH). I (2 g.) and 3.6 g. PhOH heated 14 hrs. at 110-15° in the presence of 8 drops concentrated H2SO4, the semisolid . mass poured into 50 ml. H2O, steam distilled, the residual solid extracted with very dilute NaOH, and the extract treated with dilute HCl gave IV (R = OH, 180° (2:1 EtOH-H2O with C). Similar treatment of 2 g. I and 4 g. o-cresol gave IV (R = OH, R' = Me), m. 200° (decomposition). Absorption maximum of most of the dyes were recorded as well as those of some of the corresponding dves from phthalic acid. IT 95139-41-6, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6- $(2,4,5,7-\text{tetrabromo}-3,6,9-\text{trihydroxyxanthen}-9-\text{yl})-, \gamma-\text{lactone}$ 95626-04-3, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(3,6,9trihydroxyxanthen-9-yl)-, γ -lactone 95626-20-3, 3-Cyclohexene-1-carboxylic acid, 3, 4-dimethyl-6-(1, 3, 6, 8, 9pentahydroxyxanthen-9-yl)-, γ -lactone 95626-21-4, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(3,4,5,6,9pentahydroxyxanthen-9-yl)-, γ -lactone 101200-87-7, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(3,6,9-trihydroxy-1,8dimethylxanthen-9-yl)-, γ -lactone

(preparation of) RN 95139-41-6 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid,

3,4-dimethyl-6-(2,4,5,7-tetrabromo-3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 95626-04-3 HCAPLUS
CN 3-Cyclohexene-1-carboxylic acid,
3,4-dimethyl-6-(3,6,9-trihydroxyxanthen-9yl)-, γ-lactone (7CI) (CA INDEX NAME)

RN 95626-20-3 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(1,3,6,8,9-pentahydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 95626-21-4 HCAPLUS

CN 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(3,4,5,6,9-pentahydroxyxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME)

RN 101200-87-7 HCAPLUS

3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(3,6,9-trihydroxy-1,8-CN dimethylxanthen-9-yl)-, γ -lactone (7CI) (CA INDEX NAME) HO~ Me Me Me Me CC 44 (Dyes) ΙT Dves (from 4,5-dimethyl-4-cyclohexene-1,2-dicarboxylic acid, fluorescent) Spectra, visible and ultraviolet IT(of fluorescein-type dyes from 4,5-dimethyl-4-cyclohexene-1,2dicarboxylic acid) ΙΤ 22228-48-4, 4-Cyclohexene-1,2-dicarboxylic acid, 4,5-dimethyl-(dves from) ΙT 95139-41-6, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6- $(2,4,5,7-\text{tetrabromo}-3,6,9-\text{trihydroxyxanthen}-9-\text{yl})-, \gamma-\text{lactone}$ 95626-04-3, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(3,6,9trihydroxyxanthen-9-yl)-, γ -lactone 95626-20-3, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(1,3,6,8,9pentahydroxyxanthen-9-yl)-, γ -lactone 95626-21-4, 3-Cyclohexene-1-carboxylic acid, 3, 4-dimethyl-6-(3, 4, 5, 6, 9-96172-93-9, pentahydroxyxanthen-9-yl)-, γ -lactone 3-Cyclohexene-1-carboxylic acid, 6-[hydroxybis(p-hydroxyphenyl)methyl]-3,4-96371-62-9, 3-Cyclohexene-1-carboxylic acid, dimethyl-, γ-lactone 6-[3,6-bis(diethylamino)-9-hydroxyxanthen-9-yl]-3,4-dimethyl-, 96670-74-5, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone, diacetate 97081-78-2, 3-Cyclohexene-1-carboxylic acid, 6-[hydroxybis(4-hydroxy-mtolyl)methyl]-3,4-dimethyl-, γ -lactone 101200-87-7, 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-6-(3,6,9-trihydroxy-1,8dimethylxanthen-9-yl)-, γ -lactone (preparation of) ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L83

Document No. 51:17167 Original Reference No.

1957:17167

51:3526a-i,3527a-c

Dye theory. Triarylmethane dyes of the biphenyl series. Theilacker, Walter; Berger, Wilhelm; Popper, Peter (Tech. Hochschule Hannover, Germany). Chemische Berichte, 89, 970-83 (Unavailable) 1956. CODEN: CHBEAM. ISSN: 0009-2940. OTHER SOURCES: CASREACT 51:17167. cf. C.A. 45, 7077h; preceding abstract The Ph homologous crystal AB violet carbinol (I) has been prepared and a new method for the preparation of the Ph homologous malachite green carbinol (II) is given. Fuming HNO3 (8 cc.) is added slowly to 13.2 g. (p-PhC6H4)2CO in 80 cc. concentrated H2SO4 at 5-7°, the mixture kept overnight, decomposed with ice-H2O, the precipitate extracted with boiling Na2CO3, dried, extracted with hot BuOH, and the residue recrystd. from dioxane-H2O, giving 30% bis (2, 4'-dinitrobiphenyl) ketone, slightly yellow needles, m. 223-4°. Treating 6 parts 4-02NC6H4C6H4C02H-4 (III) with 5 parts PCl5 8 hrs. with frequent shaking, and heating the mixture 8 hrs. on a water bath give 4'-nitrobiphenvl-4carbonyl chloride (IV), needles, m. 192-3°. Heating 19 g. IV in 100 cc. C6H6 with 15 g. anhydrous AlCl3 4 hrs. on a water bath, distilling the C6H6, decomposing the residue with iced HCl, and recrystg. the precipitate give 68% 4-nitro-4'-benzoyldiphenyl (V), slightly yellow needles, m. 156-7°. V is also prepared in 40% yield by heating 100 g. p-O2NC6H4Ph, 125 g. AlCl3, and 220 g. BzCl in 400 cc. PhNO2 6 hrs. at 100°, 3 hrs. at 150°, and 5 hrs. at 170°, pouring the solution into HCl (1:1), steam distilling the mixture, and extracting the precipitate with Me2CO. Reduction of V with SnCl2 in HCl at 100° gives 73% 4-amino-4'-benzoylbiphenyl (VI), yellow leaflets, m. 143-4°. Heating 2.7 g. VI, 2.6 g. anhydrous K2CO3, and 47 g. MeI 6 hrs. at 180°, distilling the excess MeI, and crystallizing the residue from H2O give 27% trimethyl(4'-benzoyl-4biphenylylammonium iodide (VII) which, thermally decomposed, gives 4-dimethylamino-4'-benzoylbiphenyl (VIII), yellow leaflets, m. 182-3°. Heating 2 g. VI, 4 g. K2CO3, and 46 g. MeI in an autoclave 3 hrs. at 210° gives 46% VII. Adding dropwise (3 hrs.) 50 g.

Me2SO4 to 7 g. VI in 75 cc. 1-C10H7Me and 75 cc. 40% NaOH heated at 160° and pouring the cold mixture into H2O give 16% VIII; from the mother liquors 45% 4-methylamino-4'-benzoyldiphenyl, m. 175°, is isolated. Heating 10 g. IV, 6 g. Ph2, and 5.2 g. AlCl3 in 90 cc.

PhNO2 1

<WALKE 10/789566><Page 168>

hr. each at 120, 130, and 140°, decomposing the cold mixture with H2O, steam distilling it, extracting the precipitate with hot dilute HCl and dilute Na2CO3, and crystallizing the residue from AcOH give 69% 4-phenyl-4'-(p-nitrophenyl)benzophenone (IX), leaflets, m. 258-9° (2,4-dinitrophenylhydrazone, red needles, m. 288-90°). Adding in small portions 4 g. IX to 170 cc. concentrated H2SO4 and 30 cc. AcOH at -5°, then adding 1.15 g. KN03 in concentrated H2SO4 and AcOH, keeping the mixture several hrs. at o°, decomposing it with ice, and washing the precipitate with KOH-MeOH and MeOH give 55% 4,4'-bis(p-nitrophenyl)benzophenone (X), light yellow needles, m. 243°. Reduction of 0.33 g. X in 100 cc. PhOMe 5 hrs. at 70° with 18 mg. used PtO2 gives 65% 4-(p-nitrophenyl)-4'-(paminophenyl)benzophenone, m. 308-10°. Reduction of 1 g. X in 170 cc. PhOMe with 55 mg. PtO2 3 hrs. at 145° gives 80% 4,4'-bis(p-aminophenyl)benzophenone (XI), yellow crystals, m. 252-4°, which is also obtained in 58% yield when 30 q. Fe shavings and 200 cc. concentrated HCl are added in small portions to 7.5 g. X in 450 cc. cyclohexanol at 140-50°, the precipitate extracted with hot C5H5N, extract diluted with H2O. Diazotizing 0.73 g. XI in 50 cc. dioxane and 180 cc. HCl (1:1) at -5° with the calculated amount of 0.5% NaNO2 solution, stirring the mixture several hrs., filtering it, adding 1 g. urea and a solution of 10 g. CuCl in 100 cc. concentrated HCl, heating it on a water bath, diluting it with H2O, and chromatographically purifying the precipitate give 4,4'-bis(pchlorophenyl) benzophenone, needles, m. 280-1°. Adding dropwise 75 g. Me2SO4 to 5.6 g. XI in 450 cc. PhOMe and 60 g. NaOH in 130 cc. H2O at 150-60°, steam distilling the mixture, and recrystg. the precipitate from PhCl give 52% 4,4'-bis(p-dimethylaminophenyl)benzophenone (XII), orange-yellow crystals, sinter 285°, m. 295-300°. Reduction of 10 g. 4-iodo-4'-nitrobiphenyl in 200 cc. cyclohexanol with 17.5 g. Fe and 125 cc. concentrated HCl gives 83% 4-iodo-4'-aminobiphenyl, m.

which (7.5 g.) is heated in 75 cc. 1-C10H7Me in a Cu flask with 50%

NaOH,

<WALKE 10/789566><Page 169>

then 35 cc. Me2SO4 added (2 hrs.), and the cooled solution poured into $\mbox{H2O}$

giving 74% 4-iodo-4'-dimethylaminobiphenyl (XIII), m. 224°. Adding slowly in a N atmospheric 2.2 g. VIII in 20 cc. tetrahydrofuran (THF) to a

Grignard reagent from 2.5 g. XIII in 100 cc. THF, refluxing the mixture $24\,$

hrs., distilling the THF, pouring the residue into NH4Cl, and keeping it $12\,$

hrs. give 3.3 g. precipitate, m. $140-60^{\circ}$, which is fractionally crystallized

from PhMe, giving 3 fractions: (a) a slightly soluble product, m. above

250° (probably a quaternary Ph derivative); (b) a dark yellow fraction,

m. 170-200°; (c) a yellow product, m. 70°. Fractions b and
c (2.5 g.) are retreated with the same amount of Grignard reagent and
the

product isolated as before giving 11% phenylbis(4'-dimethylamino-4-biphenylyl)carbinol (XIV) (Ph homologous II), yellow crystals, m. 218°; its solution in AcOH turns green on heating. Adding, in a N atmospheric, 0.9 g. finely powdered anhydrous XII to a Grignard reagent from 5 g. XIII

in 50 cc. THF, refluxing the mixture 12 hrs. with stirring, pouring the

concentrated solution into NH4Cl solution, extracting the precipitate with C6H6, and adding

cyclohexane to the extract give 0.5 g. tris(4'-dimethylamino-4-biphenylyl)carbinol (Ph homologous I) (XV), fine green-yellow crystals, m.

 $160\text{--}180\,^\circ$ (decomposition). It dissolves in H2SO4 and in HClO4 with a deep red color, in AcOH (cold) a faintly reddish brown, (hot) a deep blue

color, turning reddish brown again on cooling. The black-brown residue

from the C6H6 extraction, on recrystn. from PhCl, gives a gray-green crystalline

(putative) p,p'-bisdimethylaminoquaterphenyl, m. around 350°.
Diphenyl(4'-dimethylamino-4-biphenylyl)carbinol (XVI), prepared according to

Morton and Wood (C.A. 34, 4077), needles, m. 178-9°. The absorption spectra (AS) of XIV and XV in AcOH-Ac2O are given and compared

with those of II and I at 20, 100, and 117° , and that of diphenyl(4-dimethylaminophenyl)carbinol in AcOH; they are discussed in detail. The AS show that these color formations belongs to $\bf dye$ salts of the type of II and I.

IT 124119-87-5, Fluorescein, 2',7'-dihexyl-

(preparation of)

124119-87-5 HCAPLUS

RN

```
Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',7'-dihexyl-3',6'-
CN
     dihydroxy- (9CI) (CA INDEX NAME)
                            OH
Me = (CH<sub>2</sub>) 5
                             (CH<sub>2</sub>)<sub>5</sub>-Me
CC
     10 (Organic Chemistry)
     7285-77-0, 4-Biphenylamine, 4'-iodo- 41567-99-1, 4-Biphenylcarbonyl
ΙT
     chloride, 4'-nitro- 62750-40-7, Benzophenone,
4,4'-bis(p-aminophenyl)-
     71969-79-4, Benzophenone, 4-(p-aminophenyl)- 74974-24-6,
Benzophenone,
     4,4'-bis(p-chlorophenyl) - 94869-73-5, Benzophenone, 4-(p-
     dimethylaminophenyl) - 96711-89-6, Methanol, bis(4'-dimethylamino-4-
     biphenylyl) phenyl- 100869-70-3, 4-Biphenylamine,
4'-iodo-N, N-dimethyl-
     101884-28-0, Benzophenone, 4-(p-nitrophenyl) - 102078-74-0,
Benzophenone,
     4-(p-methylaminophenyl) - 102884-15-1, Benzophenone, 4,4'-bis(p-
     nitrophenyl) - 102884-46-8, Benzophenone,
4-(p-nitrophenyl)-4'-phenyl-
     102884-80-0, Benzophenone, 4-(p-aminophenyl)-4'-(p-nitrophenyl)-
     103166-62-7, Benzophenone, 4,4'-bis(p-dimethylaminophenyl)-
103327-17-9,
     Benzophenone, 4-(p-nitrophenyl)-4'-phenyl-,
(2,4-dinitrophenyl)hydrazone
     103401-29-2, Methanol, tris(4'-dimethylamino-4-biphenylyl)-
114791-99-0,
     Methanol, (4'-dimethylamino-4-biphenylyl)diphenyl- 117878-74-7,
     p-Quaterphenyl-4,4'''-diamine, N,N,N',N'-tetramethyl- 124119-87-5
     , Fluorescein, 2',7'-dihexyl-
        (preparation of)
ΙT
     74-82-8, Methane
```

(triaryl derivs., in preparation of dyes)